

New trends in pharmaceutical science: Bioinformatics

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The great advances in human healthcare that are presaged by the Human Genome Project can be realized by the pharmaceutical industry. A prerequisite for this will be the successful integration of bioinformatics into most aspects of drug discovery. Although, from a scientific viewpoint, this is not a difficult problem, there are formidable technological obstacles. Once these are overcome, rapid progress can be expected. Drug discovery and development is a complex, high risk, time consuming and potentially highly rewarding process. Pharmaceutical companies literally burn millions of dollars per drug to bring it to the market.

The development of a new drug requires a technological expertise, human resources and huge capital investment. It also requires strict adherence to regulations on testing and manufacturing standards before a new drug comes into market and can be used in the general population, in fact, some time it fails to come into market. All these factors just increase the cost for a new chemical entity research and development. Two branches which made positive impact on drug designing process and reduce the overall cost and risk are Bioinformatics and Pharmacogenomics. Their practice in drug designing process made positive effect on overall process and they can accelerate various steps of drug designing, and reduce the cost and over all time.

Current note focusses on the role of bioinformatics and pharmacogenomics in drug discovery and development process. Drug discovery is the step-by-step process by which new candidate drugs are discovered. Traditionally, pharmaceutical companies follow well-established pharmacology and chemistry-based drug discovery approaches, and face various difficulties in finding new drugs. Pharmaceutical companies invest heavily in all those approaches that show potential to accelerate any phase of the drug development process.

The increasing pressure to generate more and more drugs in a short period of time with low risk has resulted in remarkable interest in bioinformatics. Although bioinformatics achieved prominence because of its central role in genome data storage, management and analysis, its focus has shifted as the life sciences exploit these data.

In pharmacology, genomic, transcriptomic and proteomic data are being used in the quest for drugs that fulfill unmet medical needs, are disease modifying or curative and are more effective and safer than current drugs. Bioinformatics is used in drug target identification and validation and in the development of biomarkers and toxicogenomic and pharmacogenomic tools to maximize the therapeutic benefit of drugs. Now that the 'parts list' of cellular signalling pathways is available, integrated computational and experimental programmes are being developed, with the goal of enabling in silico pharmacology by linking the genome, transcriptome and proteome to cellular pathophysiology.

Whereas traditional bioinformatics is a wide subject it has a large focus on molecular biology, pharmaceutical bioinformatics more specifically targets chemical-biological interaction and exploratory focus of chemical and biological interactors using e.g. cheminformatics and chemometrics methods. Methods include, apart from many general bioinformatics methods, ligand-based modeling such as Quantitative structure-activity relationship (QSAR) and proteochemometrics, computer-aided molecular design, chembioinformatics databases, algorithms for chemical software, and biopharmaceutical chemistry including analyses of biological activity and other issues related to drug discovery.

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