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In Silico Pharmacology and Drug Discovery

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Short Communication

The phrase *in silico* coined in 1989 means "performed on computer or via computer simulation". It is an illusion of the Latin phrases *in vivo*, *in vitro* and *in situ* used in biology to express experiments done in living organisms, outside of living organisms, and where they are found in nature, respectively. Similarly the term "*in silico* pharmacology or computational therapeutics or computational pharmacology" explains various computational approaches available for modeling of biological processes such as biochemical, biophysical and immunological leading to therapeutic advancements. Computational approaches along with mathematical methods help to characterize the pharmacology of substances within the living organisms. *In silico* pharmacology is a growing area covering the use of software to capture, analyze and integrate biological and medical data available from different sources. The collected information is utilized to create computational models or simulations used for predictions in the discovery of therapeutics. *In silico* approaches includes quantitative structure-activity relationship (QSAR), followed by computer graphics and molecular modeling which are based on the chemistry-biology-informatics triad to bring pharmacology to new heights. Over the past 50 years, QSAR models have helped to establish connection between chemical structure and biological effects i.e. activity, toxicity, absorption, distribution, metabolism, excretion and toxicity (ADME/Tox) or physico-chemical properties. A key aspect of QSAR is use of two- and three- dimensional molecular descriptors as numerical representatives of chemical structures. The knowledge-based approach is a mean to estimate the free energies of molecular interactions in docking of ligand and protein. To ease the scoring and ranking process for molecules in large chemical libraries, QSAR concept has been extended to virtual screening to compliment the HTS and has become an integral part of today's lead discovery process. Virtual screening methods are either ligand-based or target-based, where the former considers chemical similarity at the core. The target-based approaches have been benefited with the availability of experimentally determined protein structures. Computational methods can generate predictions for pharmacological and physicochemical properties for each molecular structure and are analyzed with the help of multidimensional methods. *In silico* pharmacology uses QSAR, similarity searching, pharmacophores, homology models, other molecular modeling, machine learning, data mining, network analysis and data analysis tools based on use of a computer. The key application of these *in silico* approaches includes findings of new agonists and/or antagonists, understanding the biology, and optimization of lead molecules. These approaches helped to reduce the number of molecules made and tested, and increased speed of experiments. In conclusion, the biological systems have a highly nonlinear, even chaotic nature, whereby even tiny changes in initial conditions could make them behave in a dramatically different manner. At present we will rightly say that "No computer program will ever be able to fully model their complexity'" but in future, perhaps 50 or 100 years, when drugs will be discovered *in silico*, tested *in silico*, optimized *in silico*, and made available to patients for clinical use with little or no confirmatory testing. This is a bold and even somewhat frightening vision, but someday we will know enough about biology to go a long way towards this goal.

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