Journal of Pharmaceutical Care
jpc.tums.ac.ir

In Silico Pharmacy: From Computations to Clinics

Mehdi Soleimani[1], Mahmoud Mirzaei[1*]

[1] *In Silico* Drug Design Group, Department of Medicinal Chemistry, School of Pharmacy and Pharmaceutical Sciences, Isfahan University of Medical Sciences, Isfahan, Iran.

Received: 2017-07-25, Revised: 2017-07-26, Accept: 2017-07-27, Published: 2017-08-01.

ARTICLE INFO

Article type:
Editorial

J Pharm Care 2017; 5(1-2): 1.

► Please cite this paper as:
Soleimani M, Mirzaei M. *In Silico* Pharmacy: From Computations to Clinics. J Pharm Care 2017; 5(1-2): 1.

When calling computers, we quickly remember a complex of hardware and software to do some types of zero-one calculations through processing in the silicon hearts. In addition to several public operations, the computers could very much help the scientists and engineers to extend the borders of science and technology. From earth to space, several applications are carried out by the computers and related computational tools for various purposes. In the case of complicated biological systems, computers are also very much helpful, in which so many scientists have dedicated considerable efforts to simulate these systems to obtain more knowledge and information about the mystery of human life. There are also significant advantages of computations for the medical and medicinal applications. By developments of computational chemistry theories and soft wares in recent years, computer-aided drug design (CADD) has become a favorite technique for chemists and biochemists to design new chemical structures with higher potency of pharmaceutical applications. Besides very well known *in vitro* and *in vivo* environments, *in silico* is now a very much helpful environment for those scientists working with computer based research and development purposes of pharmaceutical laboratories and industries. The main advantage of *in silico* pharmacy is the capability of considering and examining so many chemical structures to find the lead compounds with possible pharmaceutical applications. Furthermore, lead optimizations could be very well done with various aspects of ligand based approaches to evaluate pharmacokinetic parameters. In the following, pharmacodynamics parameters of designed ligands could be evaluated by structure based approaches to find new receptors or to examine the targeted receptors for more interacting efficacy. Herein, among millions of raw chemical structures, lead compounds could be screened, evaluated and proposed for the pharmaceutical applications by *in silico* pharmacy approach. The dominant atomic and molecular scales investigations could be performed on ligand – receptor interactions to introduce new drugs for medicine. Avoiding too much use of chemicals and animals in the laboratories for *in vitro* and *in vivo* experiments and trials, *in silico* pharmacy could do all the jobs in the clean silicon heart of high performance computers to convey the new drug from computations to clinics.

* *Corresponding Author*: Dr Mahmoud Mirzaei
Address: In Silico Drug Design Group, Department of Medicinal Chemistry, School of Pharmacy and Pharmaceutical Sciences, Isfahan University of Medical Sciences, Isfahan, Iran. Tel: +983137927101
Email: mdmirzaei@pharm.mui.ac.ir