Editorial

In vivo, in vitro and in silico

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In vivo and *in vitro* are commonly used in biology and refer to experiments done in living organisms and outside of living organisms, respectively. On the other hand, *in silico* is an expression used to mean "performed on computer or via computer simulation." *In silico* was coined in 1989 as an analogy to the Latin phrases *in vivo* and *in vitro* that had been in vogue in the biological sciences for some time

In silico research in medicine has the potential to speed the rate of discovery while reducing the need for expensive laboratory work and clinical trials; this includes producing and screening drug candidates more effectively.

Using the molecular modeling technique called Protein-ligand docking, the position and orientation of a ligand (a small molecule) when it is bound to a protein receptor or enzyme can be predicted. Pharmaceutical research employs such docking techniques for a variety of purposes, most notably in the rapid *in silico* assessment of large libraries of chemical structures in order to identify those structures that are most likely to bind to a drug target, typically a protein receptor or enzyme; this helps to select likely drug candidates.

Several protein-ligand docking software applications are available, such as Autodock or EADock. There is a web service, Molecular Docking Server that calculates the site, geometry and energy of small molecules interacting with proteins.

Indeed, the protein docking algorithm EADock has been used to find potential inhibitors to an enzyme associated with cancer activity *in silico*. Fifty percent of the molecules identified were later shown to be active inhibitors of the enzymes *in vitro*. This result is far better than that of expensive high-throughput screening (HTS) which uses robotics, data processing and control software, liquid handling devices, and sensitive detectors, to quickly conduct millions of biochemical, genetic or pharmacological tests to identify active compounds, antibodies or genes for modulating particular biomolecular pathways. HTS involves testing thousands of diverse compounds a day often with an expected hit rate on the order of 1% or less with still fewer expected to be real leads following further testing.

In silico models of tuberculosis have been developed in order to aid in identifying anti-tuberculosis drug candidates within minutes rather than months. Many cellular processes are being modeled on the computer, although no exact, fully predictive, computer model of a cell's entire behavior is yet available. These limitations are a result of the limitation of knowledge not only in molecular dynamics and cell biology, but also in computer processing power.

In vitro and *in vivo* experiments have largely contributed to the much knowledge we have in the biological sciences today. The stage is set for *in silico* experimentation to throw more light on cellular processes, and contribute to the improvement of human welfare.