Bioinformatics in Drug Discovery:

Infectious diseases are now the world's biggest killers of children and young adults. The cause for this has been attributed to the unavailability of efficient drugs and if at all available, the high cost associated with those drugs. Development of cheap and efficient drugs for a disease is one of the major problems faced by mankind. The solution to this problem could be from rational drug design using Bioinformatics. The focus of the pharmaceutical industry has shifted from the trial and error process of drug discovery to a rational, structure based drug design. A successful and reliable drug design process could reduce the time and cost of developing useful pharmacological agents. Bioinformatics is the study of analysis of biological data using computer programming, mathematics and statistics.

Computational methods are used for the prediction of drug likeness which is nothing but the identification and elimination of target molecules. Drug likeness could be predicted by genetic algorithm based approaches. People have been working on constructing efficient algorithms and better energy functions to predict protein structures and interaction of small molecules with them. The technical barrier to these approaches is that they are computation intensive and we do not have the computational power to handle such massive requirement. The most important achievement of bioinformatics is the human genome project which was mapped in 2001. Bioinformatics has made it possible to sequence the genome of various organisms and there are almost hundred organisms whose genome has been mapped so far. The databases of these organisms are increasing in size day by day because every day new information about any organism's genome is gathering. The understanding of molecular biology has made it possible to design and develop the drugs. In the beginning, whole animals were used to test the synthetic organic molecules in the organ preparation. In the recent years, bioinformatics has made it easy for the researchers that they can now easily target the molecules in the in vitro environment. Now the screening of newly developed compounds can be done against the molecules of the. This way of drug development has become easy to identify the disease in an organism.

As stated earlier, from the pharmaceutical industry point of view, Bioinformatics is the key to rational drug design. It reduces the number of trials in the screening of drug compounds and in identifying potential drug targets for a particular disease using high power computing workstations and software like **Insight**. This profound application of Bioinformatics in genome sequence has led to a new area in pharmacology now being Pharmacogenomics, which is the study of genetic basis drugs response.

Drug design, sometimes referred to as **rational drug design** or more simply rational design, is the inventive process of finding new medicinal drug based on the knowledge of a biological sample. The drug is commonly an organic small molecule that activates or inhibits the function of a protein, which in turn results in a therapeutic benefit to the patient. In the most basic sense, drug design involves the design of small molecules that are rational to the biomolecule target with which they interact and therefore will bind to it. Drug designing is the modeling of such biomolecules prepared with help of bioinformatics database. This type of modeling is often referred to as **computer-aided drug design**. Finally, drug design that relies on the knowledge of the three-dimensional structure of the bimolecular target is known as **structure-based drug design**. A more accurate term is legend design (i.e., design of a small molecule that will bind tightly to its target). Although modeling techniques for prediction of binding affinity are reasonably successful.