

Drug Design In-Silico Approach for Comparative Study of Various Leads for a Specific Cancerous Cell

**Jawed Ahmed,
Ruchika Bhat,
Preetirupa Saikia**

Department of Computer Science, Jamia Hamdard, New Delhi-110062

Address for correspondence:
E-mail: jawed2047@rediffmail.com

Cancer is a deadly disease which is known to occur for various reasons. Some researches proved it to be a cause of mutations in genes, while others focused on the change in the metabolic cell division cycle as its cause. For the treatment of breast-cancer various drugs are available in market. For most of these anti-cancer drugs, mode of action is inhibiting either DNA synthesis or some other process in the cell growth cycle. In-silico approach in the field of medicine is coming up as a new tool to enhance the scope of research which is based on exploiting the knowledge of structure, pharmacophore studies, chemistry of molecules and proteins, etc.

The use of clinical trials to find the potential lead compounds when replaced with the computation & simulation techniques will not only save time but also the amount of money required for the project. We will observe the efficacy of various anti-cancer drugs through In-silico approach and compare it with practically observed results in patients. Thus the authenticity of the in-silico approach to provide large number of practically potential lead compounds could be checked. Among the various techniques used under the In-silico approach, a few of the techniques would be studied extensively to confirm the results.