**Bio-Bio-1 Capabilities in respective to Pharma Industry of Bangladesh**

**In-Silico Drug Design**

## In silico methods can help in identifying drug targets via bioinformatics tools. In silico models, a phrase used to express ‘modelling performed on computer or via computer simulation’, is an area of very active development and has great potential across the pharmaceutical industry and also in other industries, such as the consumer goods and chemical industries, where ‘non-animal alternatives’ are being actively sought for assuring the safety of chemicals.

**Homology modelling**

Homology modelling, is also recognized as comparative modelling of protein and it is a method that allows to generate an unknown atomic-resolution model of the "target" protein from its amino acid sequence and an experimental three dimensional (3D) structure of a related homologous protein (the "template").

**Molecular docking (Interaction networks)**

In the field of molecular modelling docking it is a technique which envisages the favoured orientation of one molecule to a second, when bound to each other to form a stable complex.14 Molecular docking denotes ligand binding to its receptor or target protein.

**Virtual high-throughput screening**

Virtual screening is a computational technique where large libraries of compounds are evaluated for their potential to bind specific sites on target molecules such as proteins, and well-matched compounds tested. Virtual screening plays a vital role in the drug discovery process.

**Quantitative structure activity relationship (QSAR)**

Quantitative structure-activity relationships (QSAR) methods are used to show a relationship of structural and/or property descriptors of compounds with their biological activities.

**3D pharmacophore mapping**

The 3D pharmacophore search is an imperative, vigorous and simple method to quickly recognize lead compounds alongside a preferred target.

**Molecular dynamics (MD) simulations**

MD simulations help in better understanding of biological systems. It provides time dependent investigations of protein-ligand interactions and conformational dynamics of studied complex systems.

**In Silico ADMET Test**

A good drug candidate is absorbed in required time and well distributed throughout the system for its effective metabolism and action. Toxicity is another very important factor which often overshadows the ADME behaviour. Failure of drugs at clinical trial stage due to adverse effects generated because of their toxicity proves very expensive and detrimental in the drug development process. *In silico* ADMET tools presents an array of opportunities which help in accelerating the discovery of new targets and ultimately lead to compounds with predicted biological activity.

**In silico Epitope based vaccine design**

An epitope, also known as antigenic determinant, is the part of an [antigen](https://en.wikipedia.org/wiki/Antigen) that is recognized by the [immune system](https://en.wikipedia.org/wiki/Immune_system), specifically by [antibodies](https://en.wikipedia.org/wiki/Antibody), [B cells](https://en.wikipedia.org/wiki/B_cell), or [T cells](https://en.wikipedia.org/wiki/T_cell).

**T cell epitope identification**

Consistent predictions of CTL epitopes are very important for coherent vaccine design. The most important thing is that they can reduce the wet lab experimental effort needed to identify epitopes. To elicit a T-cell immune response, proteins from pathogens and tumors must contain peptides capable of binding to the human MHC (HLA-DR) on the surface of antigen-presenting cells. Generally the more promiscuous this binding, the stronger the immune response.

**Prediction of the B-cell epitope**

Linear B-cell epitopes can predict from the immunogenic protein sequence through the B-cell epitope prediction tools of IEDB. The most significant properties for predicting B-cell epitopes are flexibility, antigenicity, surface accessibility, hydrophilicity, and linear epitope predictions. We can analyze the flexibility, antigenicity, surface accessibility, hydrophilicity, and linear epitope predictions of any antigenic protein by using the IEDB analysis resource.

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