1- Overview

The approach of drug discovery has increased considerably in the last decade. Consequently, pharmaceutical chemists and researchers have been forced to increase their knowledge base extensively and currently face a steep learning curve.

2- Aim of the In Silico Drug Discovery Lab

Target and lead discovery constitute the main components of today's early pharmaceutical research. The aim of target discovery is the identification and validation of suitable drug targets for therapeutic intervention, whereas lead discovery identifies novel chemical molecules that act on those targets. With the near completion of the human genome sequencing, bioinformatics has established itself as an essential tool in target discovery and the in silico analysis of gene expression and gene function are now an integral part of it, facilitating the selection of the most relevant targets for a disease under study. In lead discovery, advances in chemoinformatics have led to the design of compound libraries in silico that can be screened virtually

4- Requirements to held in silico drug discovery LAb:

- Computers
- Network connections
- Online resources :Protein Data Bank , Chemical Data Bank.
- Software: Online, Standalone
- Data Show

5- Applications & Benefits

- The computer-based learning course allows researchers to target their own specific studies.
- Using modern approach in research rather than the traditional routes.
- Exploring the drug receptor interactions.
- Saving time and effort to reach the new lead.
- Held regular workshops annually for postgraduate students.
- State-of-the-art technologies for hit identification
- Bioinformatics -
- Computer-Aided Drug Design
- QSAR in Drug Design
- Computational approaches for fragment based drug discovery
- Virtual Screening that helps in examining/screening millions of chemical compounds (molecules) in the Chemical Data Bank (CDB) to identify those having potential use in drug design.