**Course: Advance Bio Informatics**

**Module Title: Validation and Drugability**

**Module No: 164**

**Druggability & Validation of Targets**

It is a Post genomic era. It is a Molecular recognition & ligand binding properties of gene products. Importance of structural genomics

**Target Validation**

Disease associate target

**Disease:** alteration in protein expression

Detection of DTs by protein expression profiles Outcome & progression of disease phenotype.

**Gene-driven Initiatives**

* Disease associated & disease modifying genes
* Forward genetic screens by chemical mutagenesis
* Therapeutic targets by reverse genetic screens

**Protein Druggability**

HGP, 3000 gene loci for druggable proteins.

Sources of count INTERPRO and PFAM Computational approach

**Definition:** that can bind small drug-like compounds with high affinity and specificity.

Drug can be target via structure. Modulation of biological function not be suitable for therapeutic intervention

**Probable Binding Sites**

**Geometric-based:** Scan protein surface. CAST, LIGSIT

Ligand binding sites are concave with deep invaginations

**Energy-based:** To identify natural ligand binding site by calculating binding energies of the protein surface.