PHAMACOPHORE MODELING

PHARMACOPHORE:

IUPAC defines a Phamacophore to be a 'an ensemble of electronic and steric features that is necessary to ensure the optimal supramolecular interaction with specific biological target and to trigger or block its biological response'

(Simply, A Phamacophore model that explain how structurally diverse ligand can bind to a common receptor site.)

PHARMACOPHORE model is a hypothesis accounting for the observed biological activities of a set of molecules that bind to biological target

Phamacophore approach is a successful method sub- field of computer aided drug design (CAAD). It is essential for

1. Target identification,

2. Lead optimization, and

3. Rational design of novel drugs

Every types of group or atom in a compound reduced to Phamacophore feature (Phamacophore fingerprints). These molecular patterns would be labeled by several chemical properties such as –hydrogen bond donors of -acceptors, -aromatic, -cationic,- anionic etc. which can be used to analyze and identify the key contribution to the biological function.

Ligands:

A Ligand is a chemical substance that has the ability to bind to and from a complexes with other biomolecules in order to perform biological process

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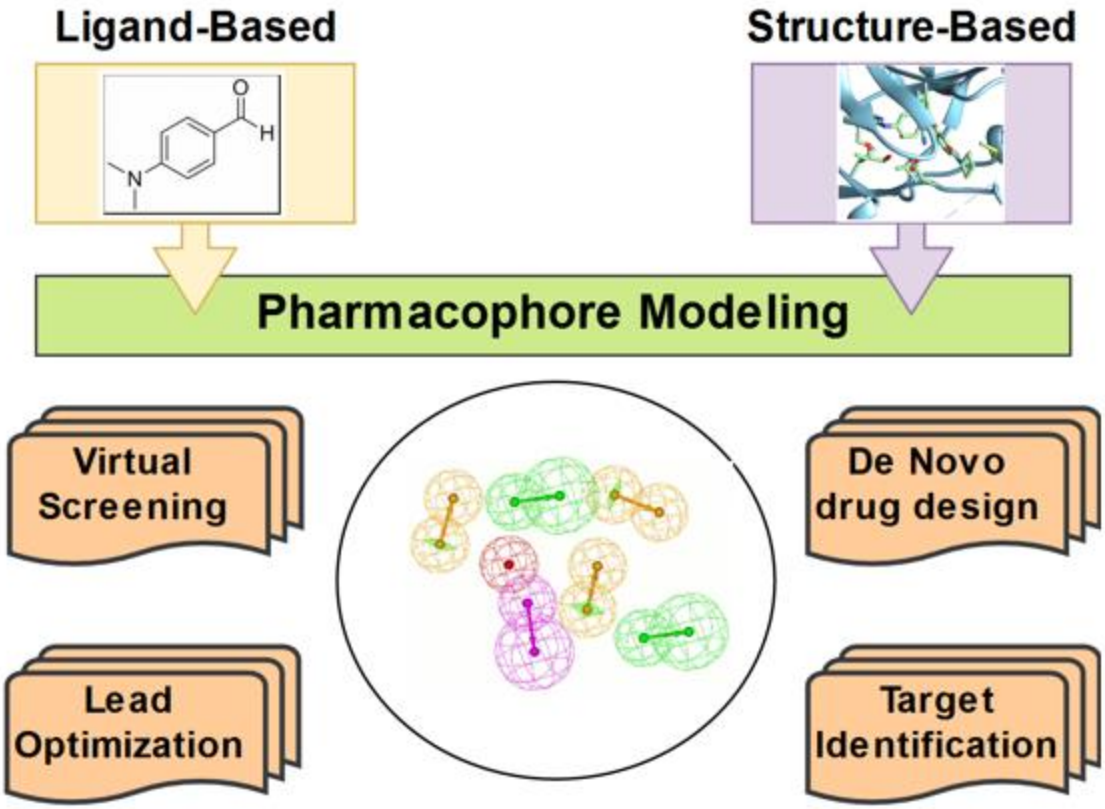

1. LIGAND BASED- PHAMACOPHORE MODELING (LBPM):

In the absence of the macromolecular target structure, ligand-based Phamacophore modeling is an essential strategy for drug discovery. In this method, the common chemical characteristics from 3D structures of multiple known ligands are extracted through ligand alignment, which would represent the essential interactions between ligand and potential macromolecular target.

2. STRUCTURE- BASED- PHAMACOPHORE MODELING (SBPM):

Structure-based-Phamacophore modeling is a method for development of Phamacophore based on the structural features of target protein. In this method the possible active sites in protein where the interactions of co-crystallized ligand occur will be analyzed