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AN ASSISTING SOFTWARES USING DRUG DESIGN

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ABSTRACT

Drug designing software's has potential role to design novel proteins or drugs in biotechnology or pharmaceutical field. The drug designing software's are used to analyze molecular modeling of gene, gene expression, gene sequence analysis and 3D structure of proteins. In addition, drug designing area has important role in the diagnosis of diseases such as lung cancer, brain cancer, breast cancer and Alzheimer disease. This review article summarizes the structure based drug designing and ligand based Drug designing software's and their applications in the field of medical research**.**

KEYWORDS: Software's, Designing, Alzheimer.

❖ ***Drug designing software's***

1) DDDPlus (Dose Dissolution and Disintegration software)

DDDPlus (Dose Disintegration and Dissolution Plus) is used to study disintegration and dissolution pattern of dosage form and active ingredients. In the formulation of new API, a single calibration experiment is generally required, after which DDDPlus predicts how changes in formulation or experimental parameters will affect the dissolution rate. This software provides precise information of dissolution and disintegration rate so it is not necessary.

Physicochemical properties of the formulation ingredients under study:
PKa's, solubility, diffusion coefficient, and density.
Particle size distribution for each of the formulation ingredients.
Interactions between the active ingredient and formulation excipients.

- **Uses**

a. Calculates the fluid velocity automatically based on the instrument speed and apparatus type.
b. DDDPlus has an optimization module that calibrates a drug's dissolution rate using a single experimental data set.

2) ***Gastro Plus (simulation software for drug discovery and development)***

Gastro Plus is a mechanistically based simulation software package that simulates intravenous, oral, oral cavity, ocular, intranasal and pulmonary absorption, pharmacokinetics, and pharmacodynamics in human and animals.

Objective function weighting is user-defined, and includes the most common weighting scheme.

- ***Uses***

a. Transporter-based drug-drug interactions.
b. Metabolic and transporter induction.
c. Linked with the industry's 1-ranked dissolution/absorption (ACAT) model.
d. Use with either compartmental or physiologically based pharmacokinetics (PBPKPlus).
e. Apply competitive and time-dependent inhibition kinetics by parent and metabolite

3) Map Check

The Map Check compare absolute dose measurements of both systems with ion chamber results. It compares IMRT QA process of Sunnuclear's MapCheck and Varian's Portal Dosimetry.

The Map Check system create verification plan for each field, export calculated dose map (Frontal) to MapCheck for each field, calibrated diode array prior to collecting data. It is user friendly software for data analysis, easier commissioning process and generates comprehensive report.

- **Uses**

a. Map Check used for IMRT verification.
b. Small detectors identify MLC.Dose based EPID IMRT QA done by using MapCheck.

❖ **Ligand interactions and molecular dynamic**

4) Auto Dock

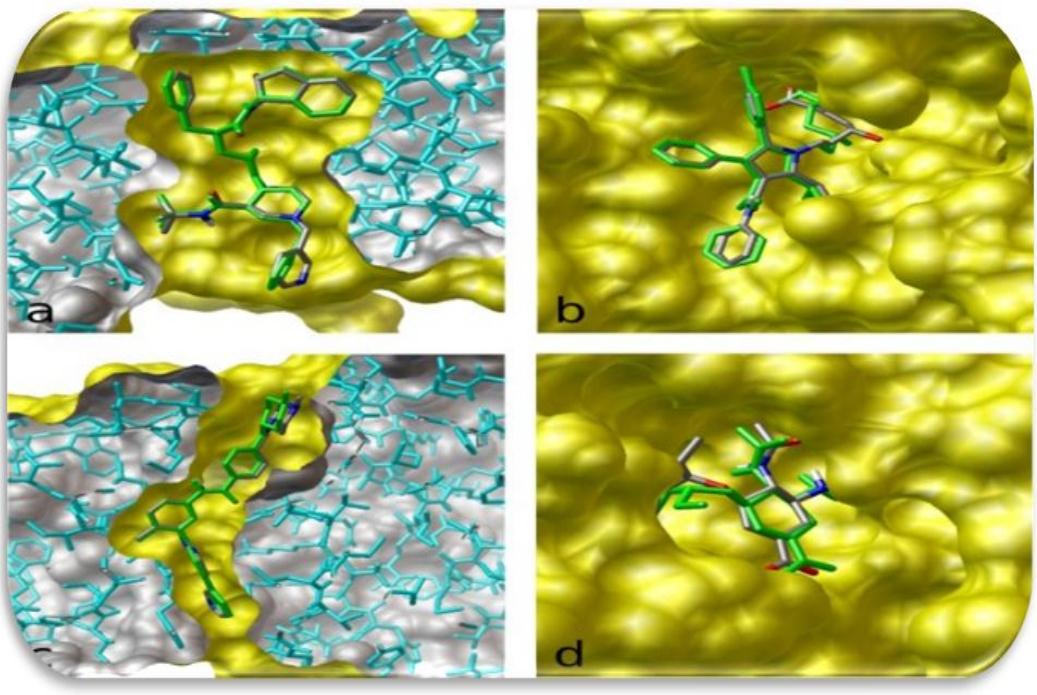
Auto Dock is an automated program employed to predict ligand and protein (bio-macromolecular targets) interactions. Continuous advancement in bimolecular X-ray crystallography helps to provide structural information of complex biomolecules such as protein and nucleic acids. These structures could be employed as targets for new drug molecules in controlling human, animal and plant diseases and disorders, and understanding of fundamental aspects of biology.

➢ **Multiple steps are employed for AutoDock calculation**

a. Preparation of coordinate files using Auto Dock tools.
b. Precalculation of atomic affinities using Auto Grid.
c. Docking of ligands using Auto Dock.
d. Analysis of results using AutoDock Tools.

- **Uses**

a. Identification of aromatic rings.
b. Used to explore the conformational states of a flexible ligand, using the maps generated by Auto Grid to evaluate the ligand-protein interaction at each point in the docking simulation.

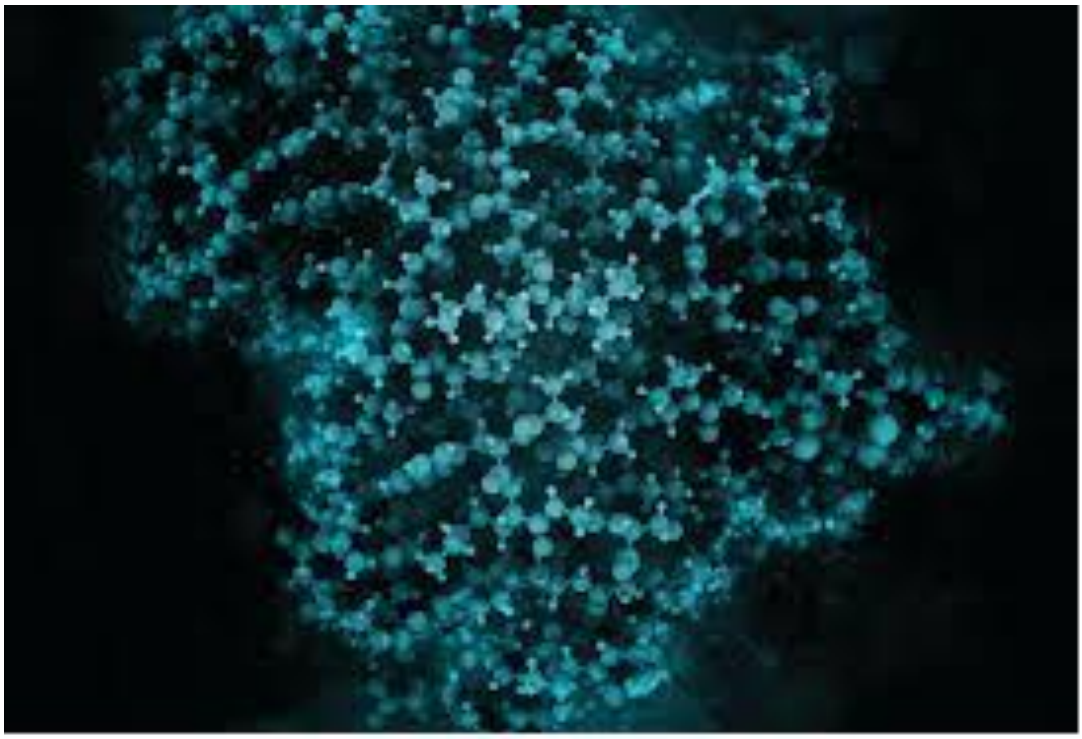


5) GOLD (Genetic Optimization for Ligand Docking)

GOLD (Genetic Optimization for Ligand Docking) is a genetic algorithm to provide docking of flexible ligand and a protein with flexible hydroxyl groups. GOLD is a part of GOLD Suite software that also includes two additional software components, Hermes and Goldmine. GOLD provides all the functionality required for docking ligands into protein binding sites from prepared input files.

The input files like the addition of hydrogen atoms, including those necessary for defining the correct ionization and tautomeric states of protein residues are obtained from Hermes. Gold Mine is a tool for the analysis and post.

Processing of docking results. GOLD will likely be used in conjunction with a modeling program to create and edit starting models.



- **Uses**

a. It is used for Protein-Ligand Docking by using Genetic Algorithm.

b. Forbidding mode predictions.

❖ **Molecular modeling and structural activity relationship:**

6) Maestro

Maestro is freely available, full-featured molecular visualization software. Maestro is a powerful tool for interpreting, managing, and sharing the results of computational experiments. It helps for building, visualizing, and sharing 3-dimensional chemical models.
It is powerful and versatile tool for the molecular modeling in the field of computational chemistry. It manages organization and analysis of obtained data.

- ***Use***

a. Quantitative structural analysis.

7) Argus Lab

Argus Lab is a molecular modeling, graphics, and drug design program for Windows operating systems. Conformational analysis such as geometry optimization study was performed on a window based computer using Argus Lab.

This software works on the principle of quantum mechanics and helps to predict potential energies, molecular structures, geometry optimization of structure, vibration frequencies of coordinates of atoms, bond length, bond angle and reactions pathway. Argus Lab calculate minimum potential energy using geometry convergence function.

Molecular docking calculations

a. It is used to build molecules.
b. Building of molecules using template structure.
c. For molecular modeling Package.

8) Sanjeevini

This software is developed to provide a computational pathway for automating lead design. It utilizes bimolecular (protein) target and a candidate drug. Software is perform identification of potential active sites, docking and scores the candidate drug and returns four structures of the candidate drug bound to protein target together with binding free energies.

In this software the drug molecule is uploaded with target protein. On uploading, software pops-up a window which displays the results of some essential pre-tests done based on the parameters needed for the acceptable format of the drug and protein files. The software

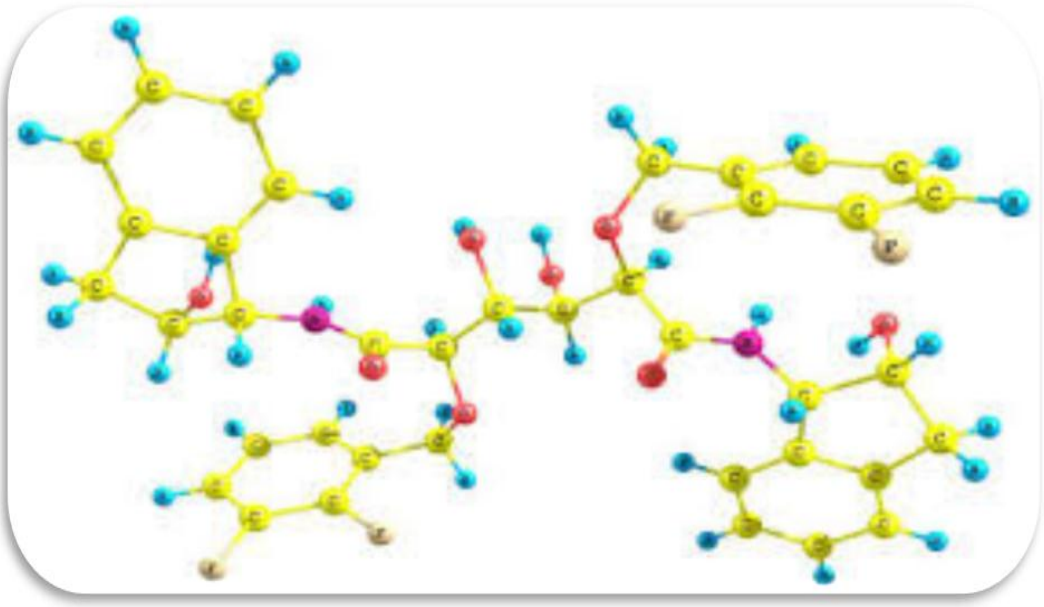
contains following modules such as Drug Preparation, Protein Preparation, Docking and Scoring, and Protein Ligand Complex.

- ***Uses***

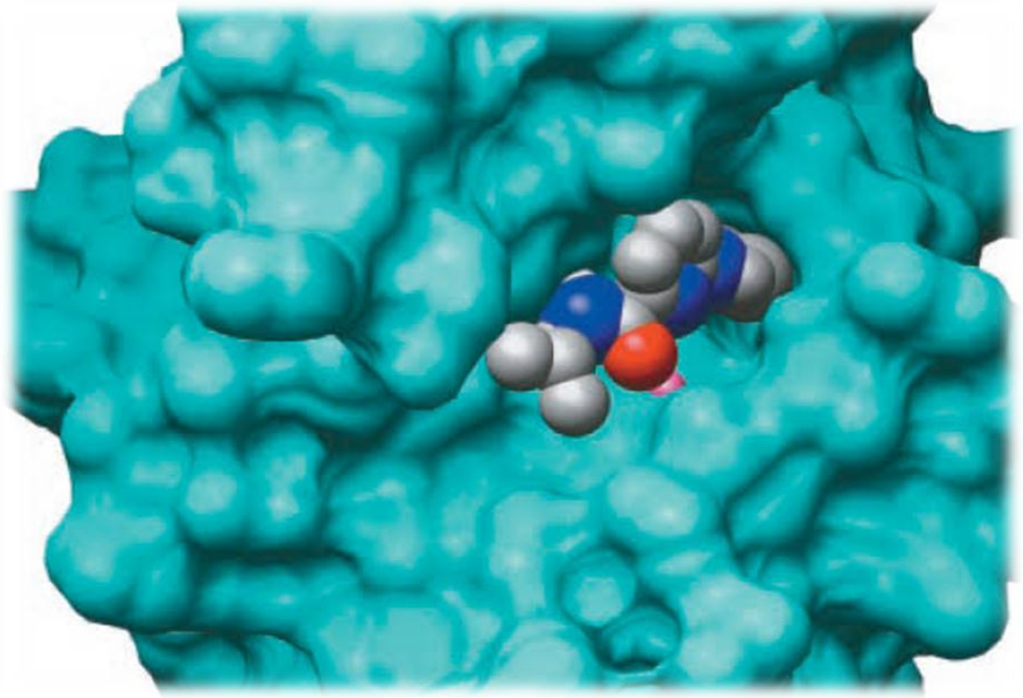
a. It is used for drug designing.

b. It predicts binding affinity.

c. Prediction of protein-ligand binding affinity.



❖ **Image analysis and visualizers**



9) AMIDE (A Medical Image Data Examiner)

AMIDE is developed in such a way that, it should provide multimodality volumetric medical image analysis. Data sets (e.g. PET, CT, and MRI) and regions of interest.

Study the root object in AMIDE, this object is used for grouping a set of related medical images and ROI's into a logical unit, and keeps track of parameters that affect the whole study.

Data set used for encapsulating volumetric medical images, this object contains the raw image data along with information needed for interpreting that data (voxel sizes, color table, thresholds, patient weight, injected dose, calibration factors, etc.).

- **Uses**

a. Provides multi-modality medical image analysis to the molecular imaging research community.

10) QSARPro

This software identify of relationship of a molecular activity or property with the structural parameters, analysis of such relationships and rapid predictions using reliable statistical modeling. It is employed to evaluate more than 1000 molecular descriptors including physicochemical, topological and electro-topological, information theory based, quantum mechanical.

It evaluate multiple options for classes of descriptors, test set, choice of linear.

- **Use**

a. Protein-protein interaction studies.

11) MARS (Multimodal Animal Rotation System)

MARS is a Multimodal Animal Rotation System which captures 360° movement of an experimental animal. The software is designed in such a way that it automatically rotates a mouse to the required positions or angels to track all the relevant molecular and anatomical information of experimental animal. It also captures optical signals generated due to orientation of experimental.

- **Use**

a. Cell tracking.
b. Enzyme activity.
c. Bone disease.
d. Inflammatory disease
e. Nanoparticle tracking and delivery.

CONCLUSION

We have discussed different software based approaches that are playing major role in the drug designing and drug discovery now days. Successful implementation of software based techniques provided an opportunity for the in vitro identification of biologically active agents, without bias towards known hits or leads. New methods such as docking also help to unravel multifarious mechanisms underlying complex target ligands interaction.

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