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Review Article **Pharmaceutical Chemistry**

A Study of Essential Computational Software in Medicinal Chemistry

Reshma R. Kurup[1*], Dr. Anoob Kumar, K. I[2], Dr. Lal Prasanth, M. L[2]

[1]B. Pharm Student, Dr. Moopen's College of Pharmacy, Wayanad
[2]HOD, Department of Pharmaceutical Chemistry, Dr. Moopen's College of Pharmacy, Wayanad

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***Corresponding author:** Reshma R. Kurup
B. Pharm Student, Dr. Moopen's College of Pharmacy, Wayanad

Abstract

Today, it is common practice to employ computational software tools for investigating the structure, dynamics, surface characteristics, and thermodynamics of inorganic, biological, andpolymeric systems. Computational software tools are a vital part of the guide for drugdiscovery. It is frequently employed in approaches for rational drug design and structure-baseddrug design. The process of drug design and discovery is essential in the invention of a new chemical entity. For this process, plenty of computational tools are available globally, Those computational software tools are fast, free, open online excess paid. Pharmaceutical software decreases human efforts, error, and time utilization in a particular task without compromising the quality of work with great accuracy and efficiency. This software is utilized by various institutes globally related to science and medicine. A computer program that transforms an input structure according toa library of medicinal chemical transformation rules beforeallowing evaluation of the output structures. High throughput screening is now widely acceptedas a viable option that CADD supports. The development of top-notch datasets and design libraries that may be optimized for molecular diversity or similarity has resulted from the questfor novel molecular entities. On the other hand, breakthroughs in computing infrastructure andmolecular docking methods are allowing screening throughput to increase quickly.

Keywords: CADD; Rational drug design; Drug discovery; Pharmaceutical software.

1. INTRODUCTION

1.1. PERSPECTIVE OF RUDIMENTARY ASPECTS OF MEDICINAL CHEMISTRY

Medicinal chemistry plays a foundational and basal role in chemical biology, and pharmacology to discover secure and effective drugs. It relies upon consecutive learning cycles composed of the compound plan, synthesis, evaluation, and information investigation to give new substance tests and lead compounds for novel and druggable targets. Using traditional methodologies, the time from speculation to acquiring the outcomes can be extended, thus limiting the number of compounds that can be progressed into clinical examinations. This challenge can be taken care of with the response of empowering advances that are showing phenomenal potential in additional fostering the medication revelation process.

Medicinal chemistry is the execution of synthetic examination approaches for the combination of drugs. During the starting periods of medicinal chemistry improvement, scientists were fundamentally worried about the separation of medicinal agents tracked down in plants. Today, researchers in this field are similarly worried about the creation of newly designed drug compounds. Medicinal chemistry is quite often equipped for drug disclosure and improvement.

Medicinal chemistry covers the accompanying stages: -

1. In the main stage new dynamic substances or medications are recognized and prepared from natural sources, natural compound responses, or biotechnological processes. They are known as a lead molecules.
2. The subsequent stage is an advancement of lead design to further develop intensity, and selectivity and reduce toxicity.
3. The Third stage is the advancement stage includes the enhancement of the synthetic route for bulk production and modification of pharmacokinetic and drug properties of a dynamic substance to deliver it synthetically helpful.

The accentuation on the improvement of the recently produced drugs has brought about the joining of various disciplines, like natural chemistry and atomic science into medicinal chemistry. These regions include biology, computer-aided design, X-beam crystallography, metabolism and pharmacokinetics, lawful and administrative issues, clinical, franchise management, pharmaceutics, and interaction research science.

1.1.1. APPLICATION OF MEDICINAL CHEMISTRY

- **Modest medications: -** Most medications utilized in illnesses are costly. Medicinal chemistry can assist with tracking down elective molecules or assembling strategies to limit the expense of the medication. This assists the medication to reach individuals of all financial situations.
- **Disclosure of new medication atoms: -** This is finished by utilizing programming where the qualitative structure-activity relationship (QSAR) is displayed.
- It presently utilizes computer-aided drug discovery (CADD) to limit the time taken for the drug revelation process.
- It evades the need to synthesize all the test particles and test them on numerous animals. By the utilization of CADD, the medication molecule and its capacity to deal with a receptor are anticipated.
- **Minimal harmfulness: -** Any medication we take is an unfamiliar substance to the body. So, the medication arranged should be safe for the body and ideally less harmful Medicinal chemistry endeavors to get ready water-dissolvable medication particles that will be effectively utilized. Or on the other hand, if lipid solvency is wanted, the atom which can undoubtedly be switched over completely to water-solvent structures is made. In this way, the aggregation of the toxic substance of the medication is constrained.
- It assists with creating successful meds, limiting harmfulness, and economically producing the medication.

1.2. LEADING OUTLOOK ON DRUG DESIGN AND DEVELOPMENT BASED ON MEDICINAL CHEMISTRY

The process of drug discovery and development is very convenient with the invention of various computational software and tools. Drug design and discovery are usually made by using computer software for virtual screening by structure or ligand-based design and lead optimization. There is also some computer software available for structural affinity by selective structure-based design and lead optimization of some physicochemical properties for the improvement of drugs.

Drug design and discovery approaches include combinatorial chemistry, biology, high- throughput screening, and drug metabolism (ADME) groups, which are linked together. A lot of computational software or tools are available worldwide for drug design with different uses, accuracy, and precise techniques. Computational tools are essential for lead optimization, lead discovery, and pre-clinical in vitro examination criteria for initiating clinical development.

Computational tools are essential for Computer-aided drug design because these processes are a cost-effective, reliable, and time-saving technique. Novel drug discovery and design are widely used in different techniques such as rational drug design and structure-based drug design. Computer-based drug design has completely changed the way new drugs are discovered since it is quicker, cheaper, and has more effective pharmacological action. Computer-Based Drug Design is primarily used for drug design and has had great success in the development of novel drugs.

1.3. COMPUTER-AIDED DRUG DESIGN (CADD): AN IMPENDING APPLIED SCIENCE FOR DRUG DESIGNING

Computer Aided Drug Design (CADD) and Delivery Systems provide an in-depth analysis of the computer-assisted techniques used to discover, design, and optimize advanced, efficient, and intact drugs. Computer-aided design is being utilized to promote and facilitate hit identification, hit to lead selection, streamline the assimilation, circulation, digestion, discharge, and toxicity profile, and evade safety issues. The computer-aided drug design (CADD) has impressively broadened its reach of utilizations, crossing practically all stages in the medication disclosure pipeline, from target recognizable proof to lead disclosure, from lead enhancement to preclinical or clinical preliminaries The expansion of computer-aided drug design technologies to the R&D accession of an association could lead to a depletion in the cost of drug design and progress by up to 50%.

Given the accessibility of the 3D construction of the objective protein, CADD methods are assembled into two types –

- Structure-based drug design {SBDD}
- Ligand-based drug design {LBDD}

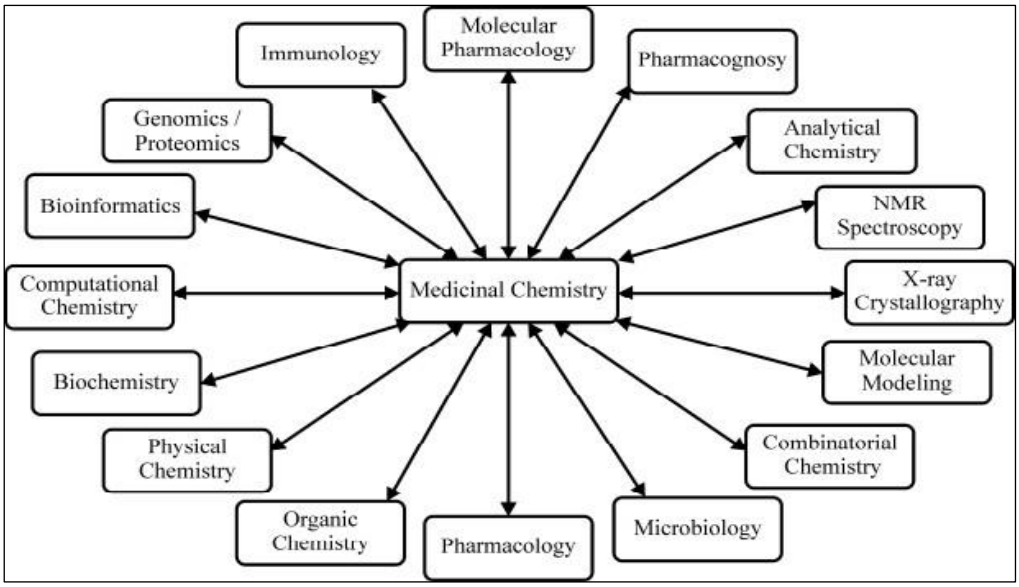

Figure 1.1: Branches of Medicinal Chemistry

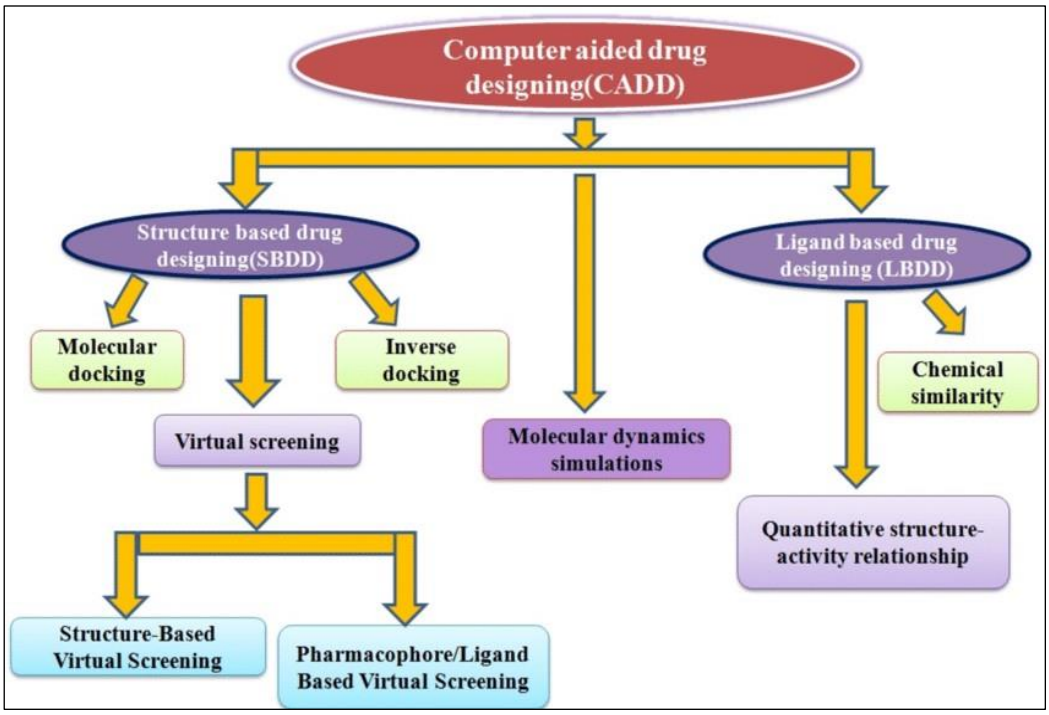

Fig 1.2: Types of CADD

1.3.1 ROLE OF CADD

The objective of CADD isn't to track down the best medication but to recognize and improve lead mixtures and save a few tests.

The boundaries anticipated from medication are: -

- Effectiveness
- Solidness
- Innovation
- Feasibility

1.3.2. LIMITATION OF COMPUTER-AIDED DRUG DESIGN

- Tedious
- Expensive
- Intellectually unrefined

1.3.3. FUTURE RESEARCH ACTIVITIES

- Biomolecular stimulant investigations of proteins, sugars, and DNA.
- Forecasting of free energies of binding and restoration.
- QM/MM studies of the consolidated stage.
- To study prospective interchange with other proteins or nucleic acids.
- Improvement and use of computational methods for forecasting binding and salvation.
- Improvement and use of new techniques for

starch computational science.

- Understanding how groups of ligands dock into restricting locales of macromolecules.

1.3.4. APPLICATION OF COMPUTERS IN DRUG DESIGN

- Target catalyst
- Drug transport
- Biochemical transformation
- Structure assurance of protein
- Molecular similarity

1.4. EXPLORATION OF SOFTWARE

Software is a computer program and related data that lay out the instructions for the computer to perform tasks. Software programs used in pharmaceutical sciences are concerned with the vast subject regions such as pharmacology, pharmaceutical chemistry, and pharmaceutics. pharmacognosy, and pharmaceutical biotechnology. Computational methodologies, for example, docking give connections to small molecules with underlying macromolecules and accordingly hit recognizable proof and lead to streamlining. These strategies are quicker, and precisely give significant experimental findings and activity of components. Likewise, the execution of these methods could prompt a decrease in the cost of medication planning and improvement. At present in biomedicine sciences, these software programs are showing a crucial role in the various periods of medication revelation and planning strategies.

Software programs that help to process the data as wanted. There are 2 major kinds of software programs: -

- **SYSTEM SOFTWARE: -** It helps the computer to run its resources.
- **APPLICATION SOFWARE: -** It is the ‘’end-user’’ software.

The expedition of software and model-based tools has become a crucial element of drug discovery and evolution in the pharmaceutical industry, which plays a pivotal role in broadening advanced bioactive drugs beyond a spectrum of therapeutic regions. Significant expense, deficient and extended time term, an elevated degree of chance, a vulnerability in the outcomes, and profoundly complex methodology are the primary difficulties in the advancement of a new drug. To conquer these issues, it is expected to utilize new and more efficient drug uncovering and planning strategies.

Novel Software-based techniques such as molecular modeling, structure-based drug design, structure-based virtual screening, ligand interaction, and molecular dynamics are dominant tools for the disquisition of pharmacokinetic and pharmacodynamic attributes of a drug and structural activity relationship between a molecule and its target.

1.5. PREVAILING AND EXCEPTIONAL APPLICATION OF SOFTWARE

Software used in pharmaceutical chemistry is to clarify various physiological properties of drugs and to predict activity values for advanced compounds within certain limits. They may be extensive assistance to those trying to generate considerable databases from a massive attempt in drug research.

- Proper utilization of programming and computer-based modern approaches has reduced several interruptions in the process of drug discovery and hastened new drug development. Further develop efficiency and explain time-consuming manual tasks.
- Measurement of dosage regimens in hospitalized persons with renal failure.
- Inspecting, examination, quantization, data handling, and reporting are all performed by the computer according to the analysis parameters.
- The computer-based programs fundamentally record the estimations compared with standards and transmits signals to controlling devices to make the vital changes.
- For the further development of the drug store programming in the market today.

1.6. SOFTWARE FOR DRUG DESIGNING, DISCOVERY, AND DEVELOPMENT

The software is further categorized based on the task executed by the software and its working principles like software estimating pharmacokinetic parameters, ligand interactions, molecular dynamics, molecular modeling and structural activity relationship, image analysis and visualizers, and data analyzer and behavior analysis software.

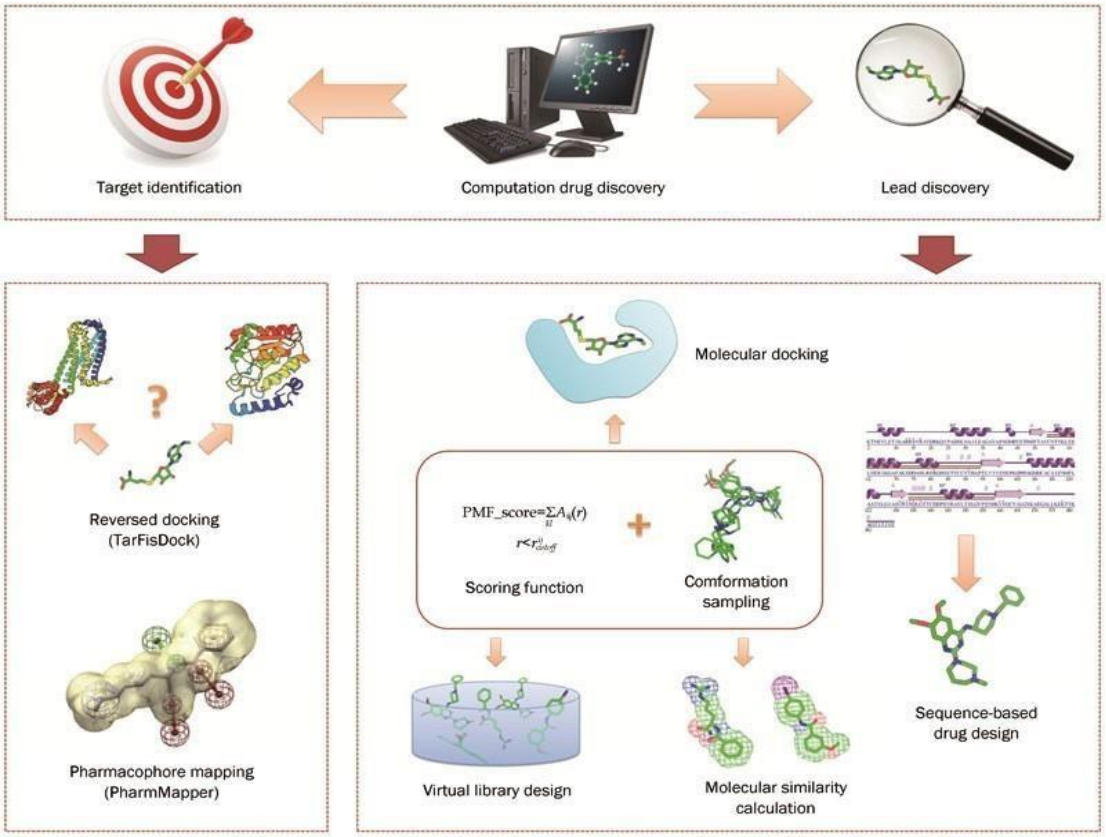

Fig 1.3: Sources and resources of medicinal chemistry

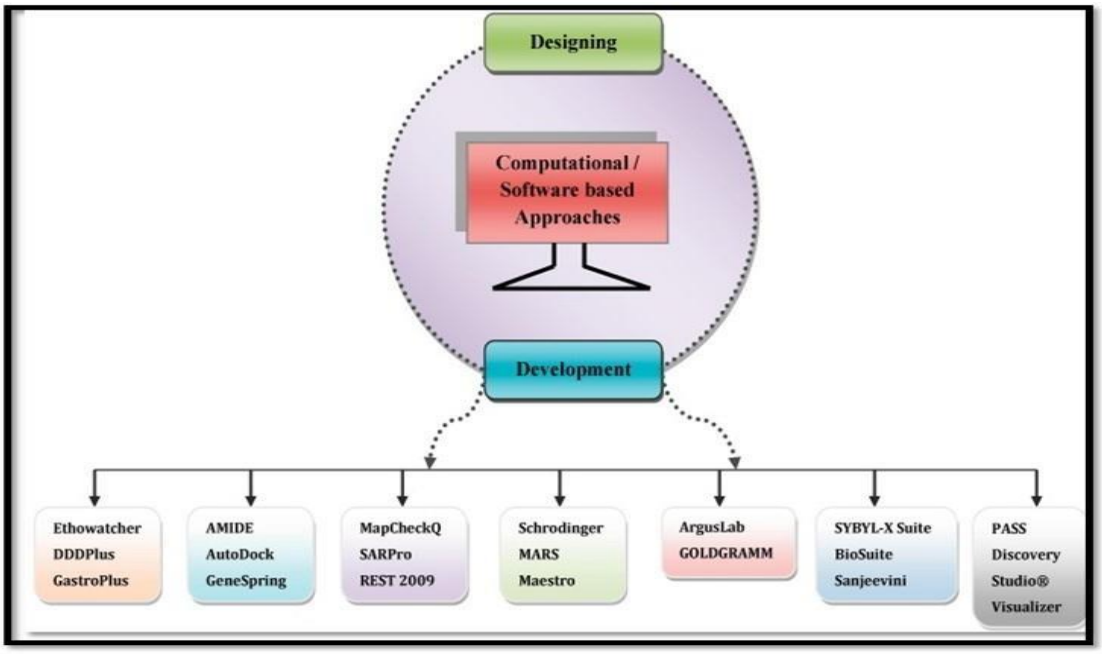

Fig.1.4. Software-based approaches for drug designing and development

2. REVIEW OF LITERATURE

1. Mahaveer Prasad Kabr *et al*., (2013) explained that Software is a computer program and related data that provide instructions to the computer to perform a particular task. These programs are designed to address special-purpose applications. Applications of software in pharmaceutical chemistry are to elucidate various predicted activity values for new compounds within certain limits. They may be of enormous assistance to those trying to generate large databases from massive efforts in drug research.
2. Prasad G. Jamkhande *et al*., (2017) outlined that Drug discovery including drug designing and

development, is a multifarious and expensive endeavor, where the least number of drugs that pass the clinical trials make it to market. Software-based drug discovery and development methods have had a major role in the development of bioactive compounds over the last three decades. This review discusses the working principles and successful applications of the most commonly used software for drug designing and development.

3. Jimish R. Patel *et al*., (2020) summarized that in the current era of modern drug design & and development via computer-aided drug design, the potential role of computational software tools is widely enlarged in use. Computer-based drug design is revolutionary in the new drug discovery process because these processes are fast, time, and cost-saving with more efficient pharmacological activity. Computer-based drug design is mainly applied for the design and has many successes in new drug research.
4. Antimo Gioiello *et al*., (2020) explained that Medicinal chemistry plays a fundamental and underlying role in chemical biology, pharmacology, and medicine to discover safe and efficacious drugs. Small molecule medicinal chemistry relies on iterative learning cycles composed of compound design, synthesis, testing, and data analysis to provide new chemical probes and lead compounds for novel and druggable targets.

3. ESSENTIAL SOFTWARE IN MEDICINAL CHEMISTRY

The significant utilization of software in unadulterated science is for QSAR. It is feasible to clarify the impact of different physiological properties of drug intensity furthermore, to anticipate new compounds within certain limits. QSAR innovation utilizes complex computers, atomic illustrations, and complex programming. They might be of tremendous help to those attempting to produce the enormous data sets resulting from massive endeavors in drug research.

Software-based approaches are playing a significant part in medication planning and medication revelation nowadays. Successful execution of programming-based procedures which provide a chance for the in vitro identification of biologically active agents, without inclination toward known hits or leads. New techniques, for example, docking additionally help to disentangle diverse mechanisms of fundamental complex objective ligands collaboration. Huge advances and utilization of new programming projects keep on being made in the field of pharmacokinetics and pharmacodynamics are benefitting the procedure of drug discovery. This understudy upgrades drug revelation and costs the hardships of the few biochemical businesses. Programming-based approaches can be sure to be utilized to help the exorbitant, complex, and highly challenging drug planning and discovery process.

There is specific programming such as: -

DRAWING SOFTWARE: -

a) CHEMSKETCH
b) CHEMDRAW
c) MDL-ISIS

NOMENCLATURE SOFTWARE:

d) AUTO-NOM

TOXICITY PREDICTION: -

e) DEREK

ADME: -

f) MOLINSPIRATION
g) SWISS
h) PASS ONLINE

3.1. DRAWING SOFTWARE: -

a) CHEMSKETCH

- It is a molecular modeling program used to create and modify images of chemical structures.
- There is another software {CHEM-3D} which is used to display the two and three dimensions of molecules.
- To understand the nature of the functional groups and structure of the chemical bonds.
- Based on modified molecular mechanics, it takes into consideration non-bonded interactions such as Van der Waals, internal rotation, bond stretching, and angle bending.

ASPECTS:

- The program offers a few advanced features that allow the molecules to rotate and apply color to visualization.
- It has a few layouts with particles and functional groups with the possibility to add text and utilize different instruments to streamline creations made by the software.
- Generate IUPAC Names.
- Calculate Molecular Properties.
- Search for Structures.
- The 3D view is the best feature of Chemsketch which is used to visualize chemical structures in a 3D mode in different formations like wireframes, balls & sticks, space fill, disks, and dotted structures with different backgrounds.

IMPLEMENTATION:

- Easy to draw structure.
- Easy to understand.
- Tells us about the whole properties of the structure.
- To view them as 3D models.
- It can be used to visualize the structures of organic molecules, names of an organic

molecule as well as Lewis's structure.

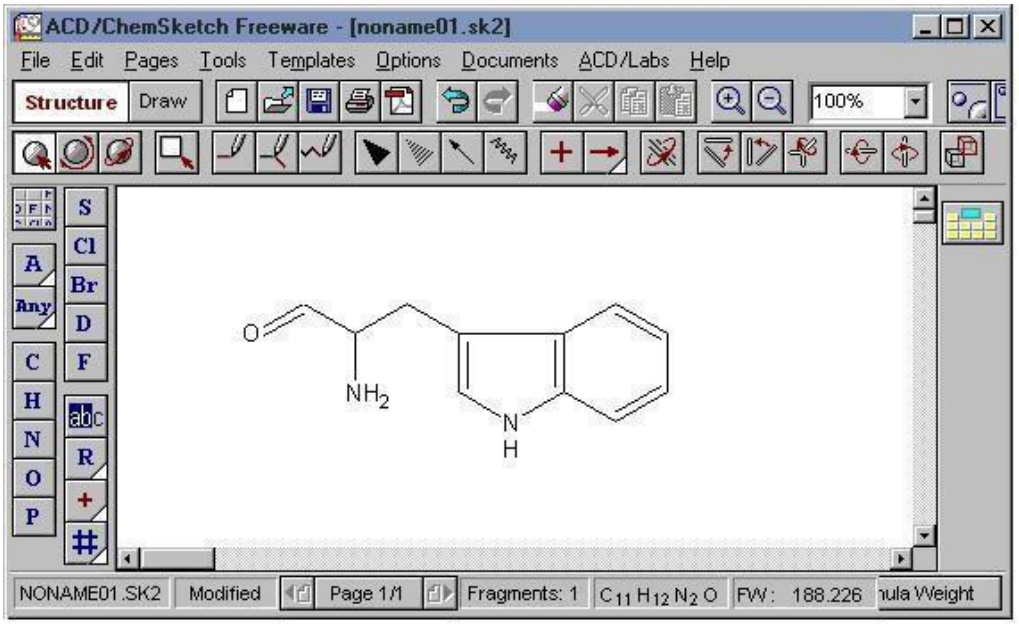

Fig 3.1: Structure Drawing

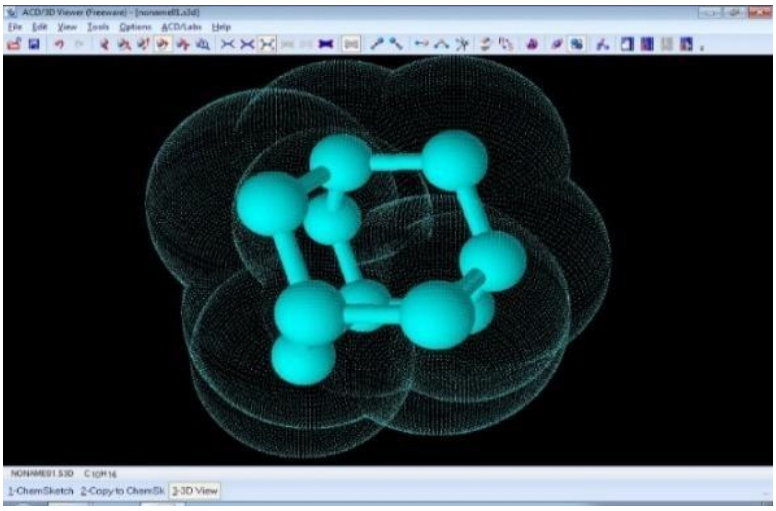

Fig 3.2: Ball and stick model

b) CHEMDRAW

- Chemdraw is a program for PCs that helps you draw molecules and other chemical images such as equations and lab apparatus.
- It is a chemistry software that helps us in many chemical structures.
- It can convert the name of a molecule into its structure and vice versa.

ATTRIBUTES: -

- Chemical name to structural conversion
- NMR Spectrum stimulation
- Mass Spectrum stimulation
- Chemical structure to name conversion
- Draw ligand structure

IMPLEMENTATION:

- Users can also use it for the prediction of properties and spectra, convert chemical structures to IUPAC names
- Chemdraw is a drawing program that enables users to depict biological entities and biological processes in addition to chemical structures and reactions.
- It can be used to visualize 3D structure

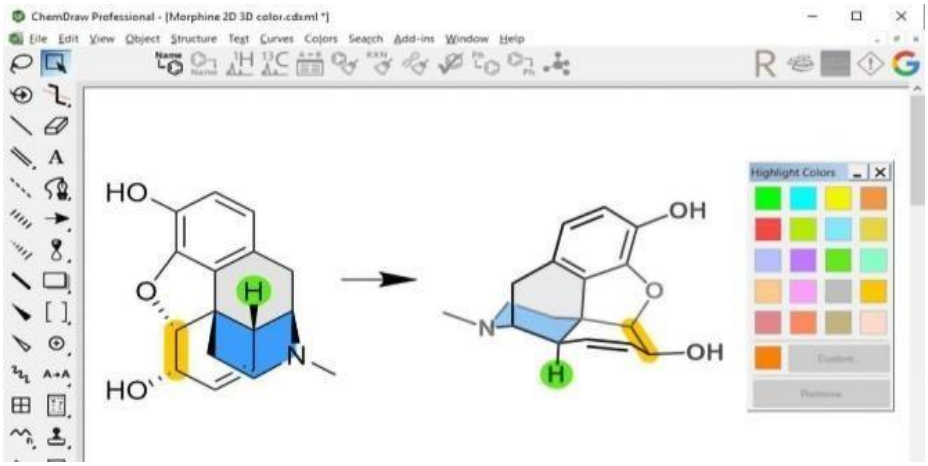

Fig 3.3: Morphine 2D & 3D color form

c) MDL-ISIS

- An integrated scientific Information system serves as an information management framework for the discovery of data.
- It has extensive chemical representation features or powerful chemical structures, either a chemical reaction or the ability to search 3D models.

IMPLEMENTATION:

- ISIS is also an application development environment that allows extending software beyond chem drawing and databasing to managing chemical inventories, creating electronic lab journals, and managing therapeutic level lead candidates.

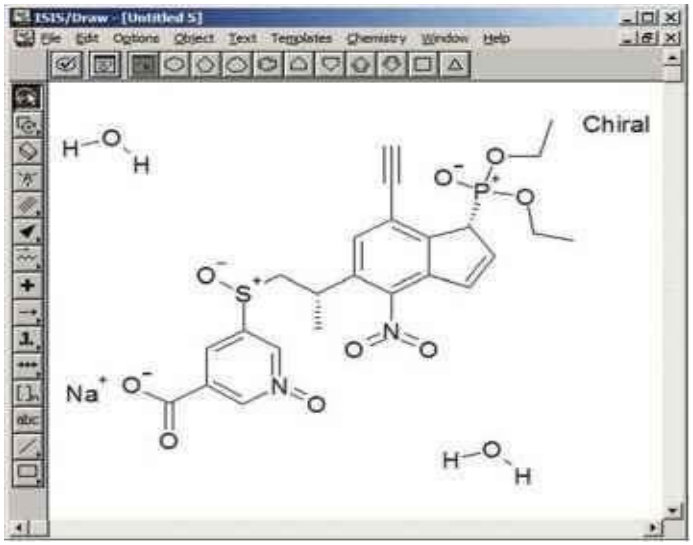

Fig 3.4: ISIS/Draw

3.2. NOMENCLATURE SOFTWARE: -

d) AUTONOM

- AUTONOM (Automatic Nomenclature) is a fully automatic, practical system for creating names directly from structural diagram input of organic compounds.
- It is a chemical naming software system for Windows and Macintosh Operating systems.
- It uses a proprietary algorithm based on IUPAC nomenclature rules to generate IUPAC names automatically from chemical structures.
- The IUPAC procedures for giving structures systematic names are complicated and usually result in the selection of numerous non-unique names.
- AUTONOM is software to overcome these difficulties by using algorithms to the structure diagram of the compound and generate a unique IUPAC-compatible name.

ATTRIBUTES:

- Chiral interpretation (R & S Configuration)
- Double bond topology (E, Z descriptors)
- CAS ring system naming conventions support
- Ability to number atoms within the named structure

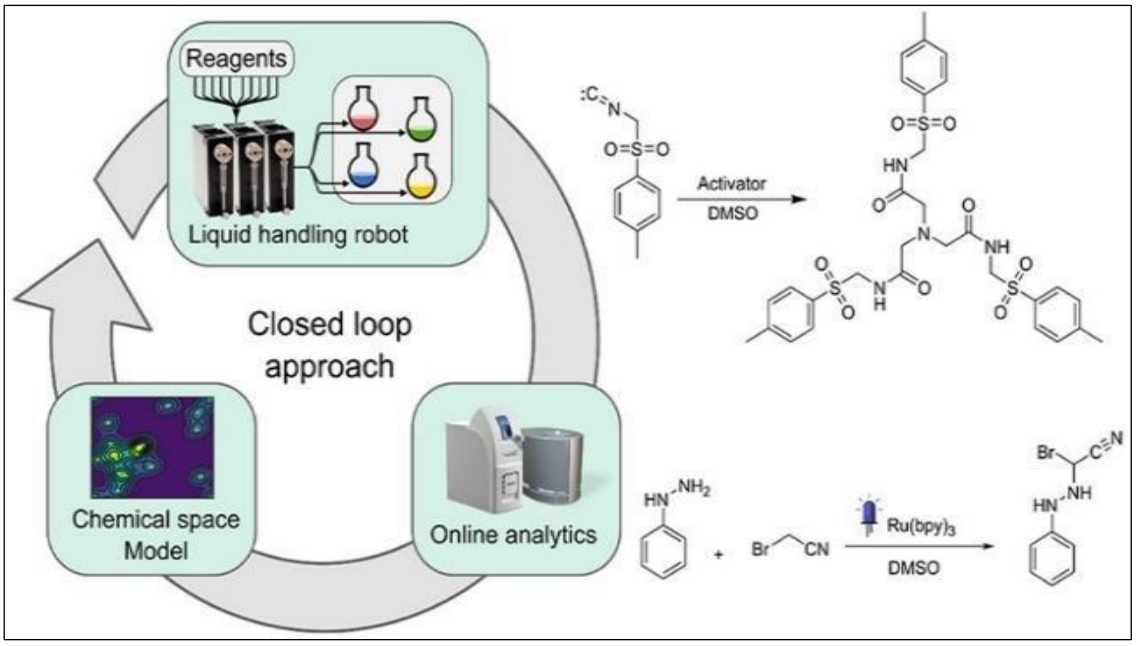

Fig 3.5: Autonom software process

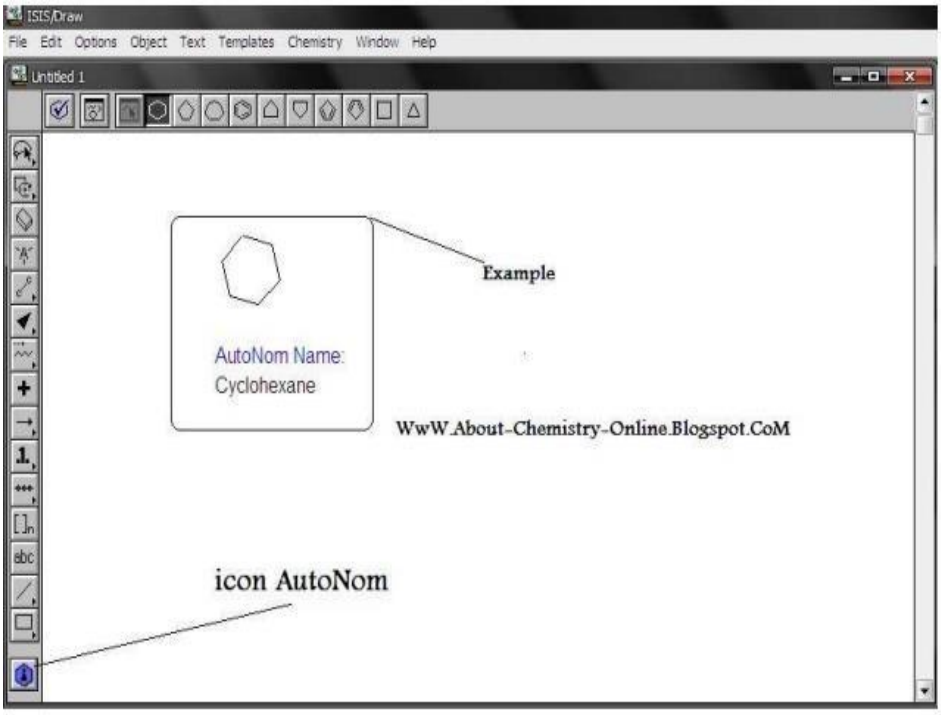

Fig 3.6: Autonom Software

3.3. TOXICITY PREDICTION:

e) DEREK

- It is a rule-based expert system that predicts toxicological hazards of chemicals, based on an analysis of their molecular structure.

ATTRIBUTES:

- It utilizes the Structure-activity relationship (SAR)
- It considers physicochemical properties to derive its prediction

IMPLEMENTATION:

- It is an expert, knowledge-based software that gives fast and accurate toxicity predictions

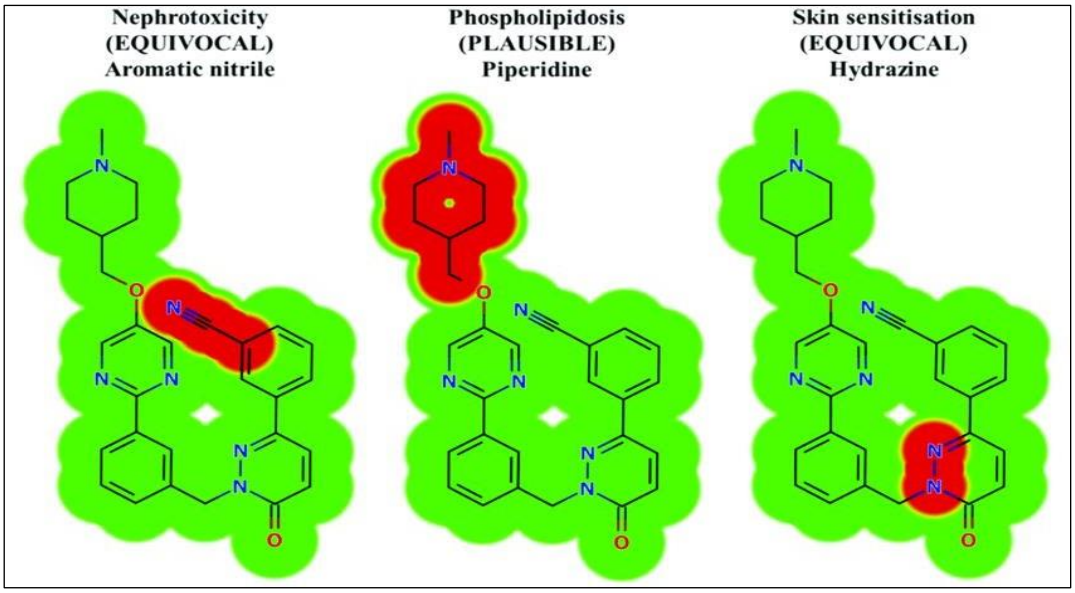

Fig 3.7: Derek Software toxicity prediction

3.4. ADME:

f) MOLINSPIRATION

- Molinspiration is an independent research organization focused on the development and application of modern cheminformatics techniques.
- Java-based cheminformatics software is the area of expertise of Molinspiration.

❖ **ATTRIBUTES:**

- Normalization of molecules
- Generation of tautomer
- Molecule fragmentation
- Calculation of various molecular properties needed in QSAR
- Molecular modeling and drug design

ϖ **IMPLEMENTATION:**

- It allows visualization of molecules and related numerical data
- Easy data mining.

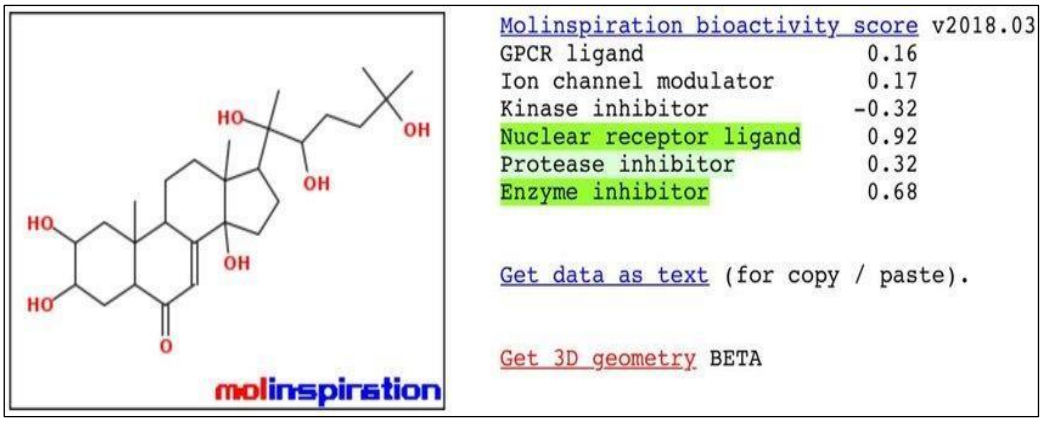

Fig 3.8: Molinspiration software

g) SWISS

- This website allows you to compute physicochemical descriptors as well as to predict ADME parameters, pharmacokinetic properties, drug-like nature, and medicinal chemistry friendliness of one or multiple small molecules to support drug discovery.
- Free access is provided through the SwissADME web service to a collection of quick yet reliable prediction models for physicochemical attributes, pharmacokinetics, drug- likeness, and medicinal chemistry friendliness.

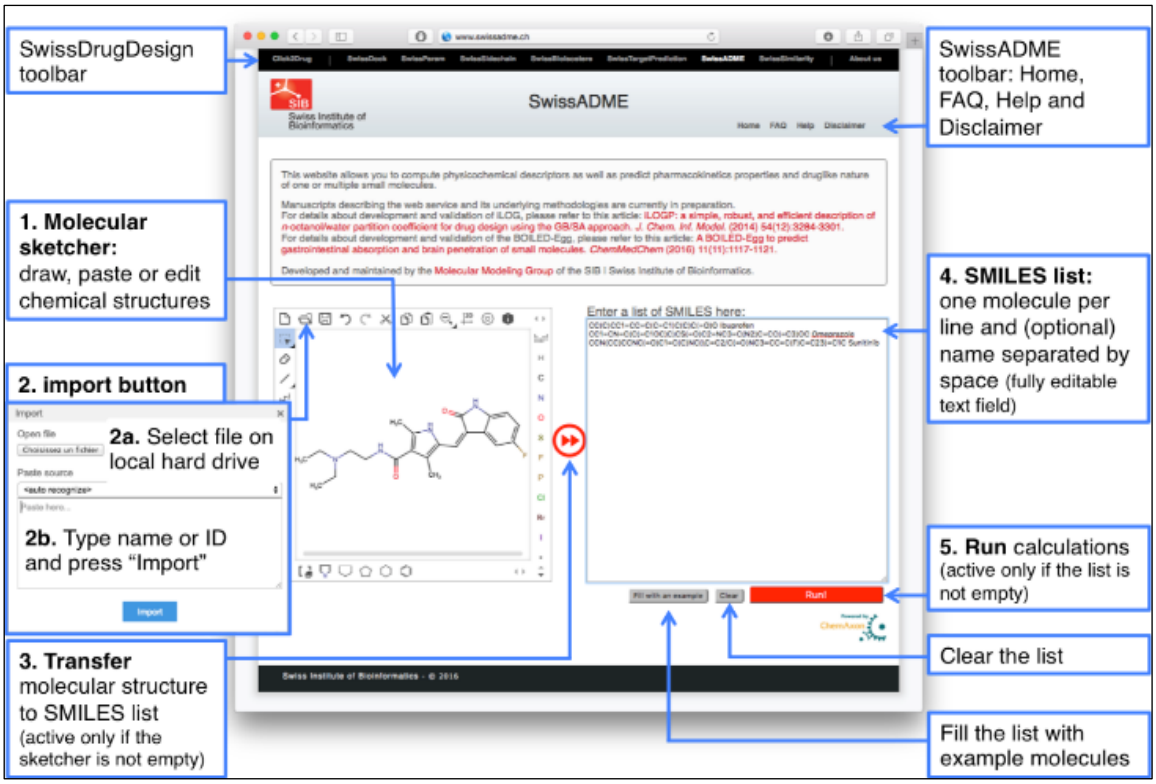

Fig 3.9: Swiss ADME

h) PASS ONLINE

- ASS Online predicts over 4000 kinds of biological activity, including pharmacological effects, mechanisms of action, toxic and adverse effects, interaction with metabolic enzymes and transporters, influence on gene expression, etc.

ϖ IMPLEMENTATION

- To obtain the predicted biological activity profile for your compound, only a structural formula is necessary; thus, prediction is possible even for a virtual structure designed in a computer but not synthesized yet.

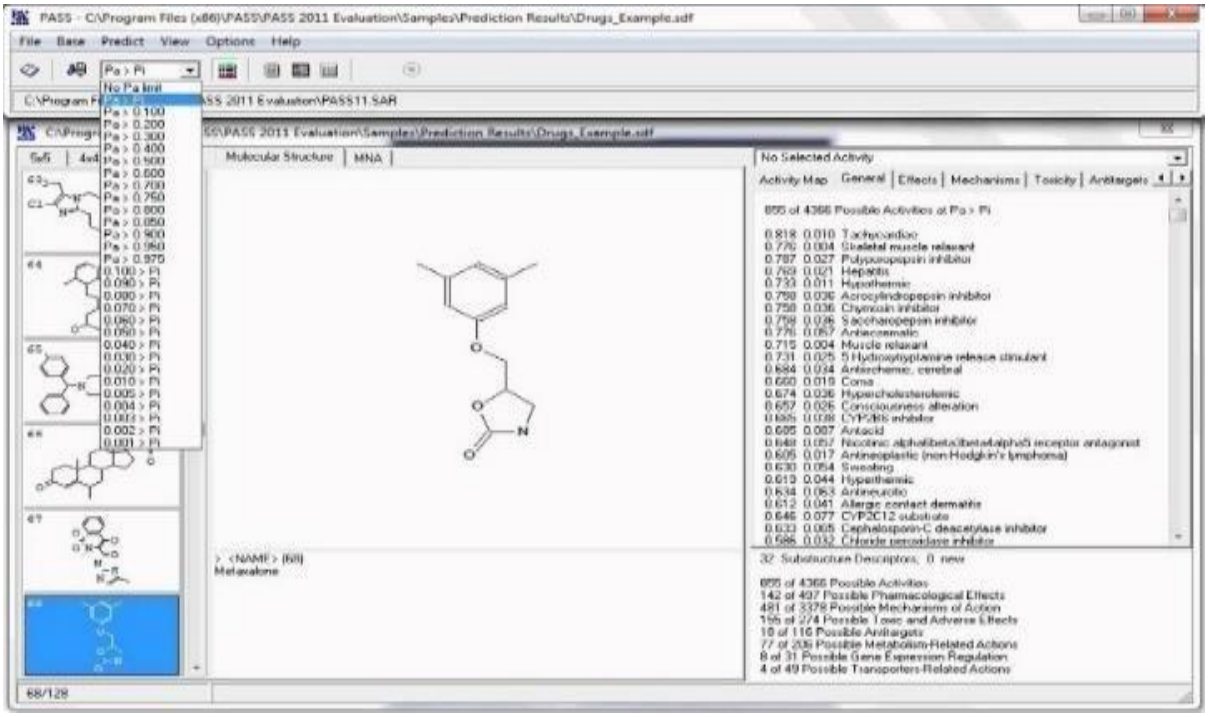

Fig 3.10: Pass Online Software

4. DRUG DESIGN SOFTWARE

A computer needs software for its capabilities like projects. This software simplifies our work and is quicker. Different organizations, for example,

- AUTODOCK
- GLIDE

a) AUTO DOCK

- Auto Dock is a suite of automated docking tools.
- It is intended to forecast the interactions of tiny molecules, such as substrates or potential medications, with a known 3D structure of a receptor.
- Auto Dock is a valuable docking program where the docking score of known 3D structure with target protein can be acquired regarding affinity.

❖ **ASPECTS: -**

- Receptor adaptability
- Blind-docking
- Precalculated lattice maps on a limiting site
- A great relationship between predicted inhibition constants and trial information

❖ **IMPLEMENTATION: -**

- To screen different potential mixtures
- Discovering novel substances with certain binding characteristics
- Testing a scope of changes of a current compound.

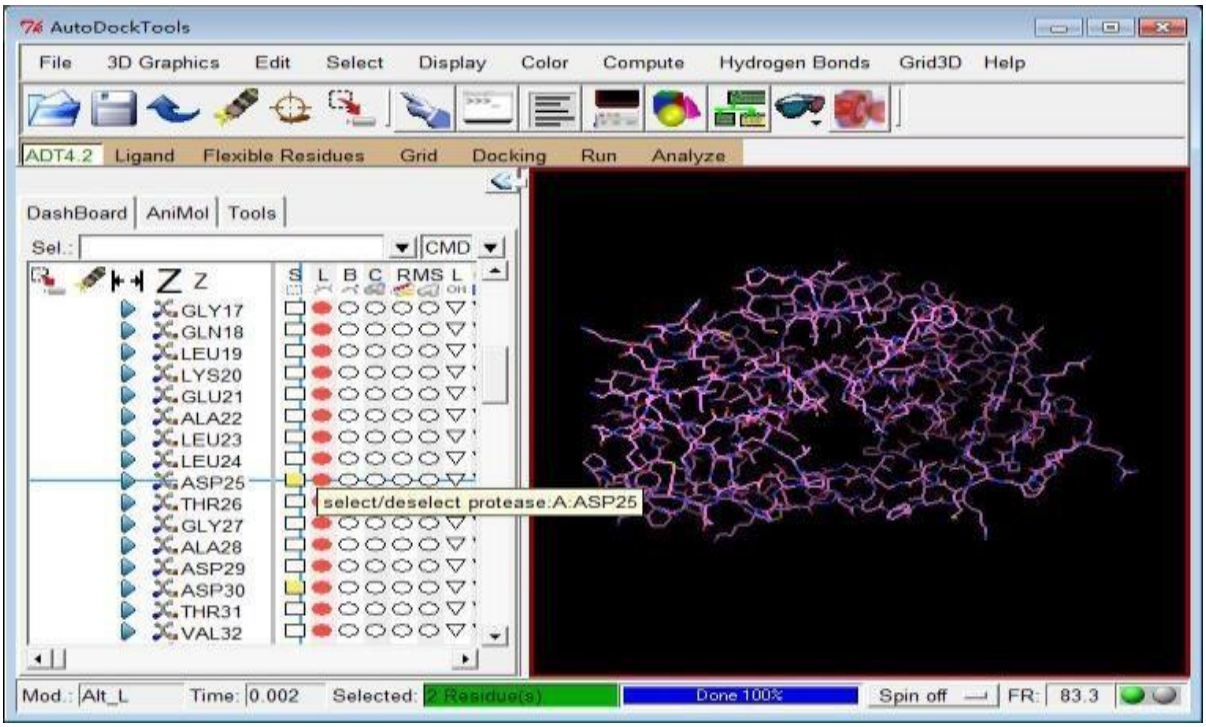

Figure 4.1: Auto dock

b) GLIDE

- It is another type of QSAR software.
- It is under the control of Schrodinger.
- Mainly used for docking techniques.
- The docking procedure mainly helps in understanding the action of the drug on the molecular level.
- The process of the action of the drug in our body mainly starts with its binding to specific enzymes, which further helps in catalyzing the drug's action.
- The drug binds to the active site of the enzyme, the extent of binding of the drug to the enzyme is generally related to its extent of action.

❖ **IMPLEMENTATION: -**

- This software gives a score, which determines the extent and efficiency of the binding ability of a drug.
- Thus, the scores of established drugs are fed to the software. When a new analogue of the drug is found, its score is compared with the score of the standard for the particular enzyme.
- If the score is greater than that of the established drug, then it can be assumed that the new analogue has better action than the established drug, at least at the molecular level.

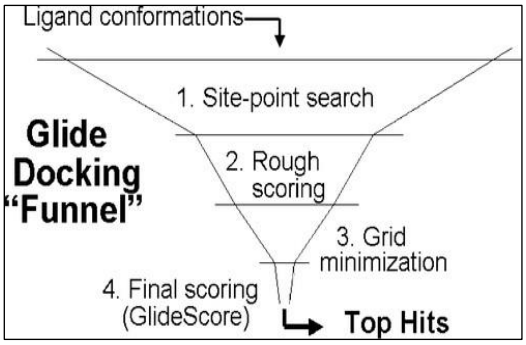

Fig 4.2: Glide docking funnel

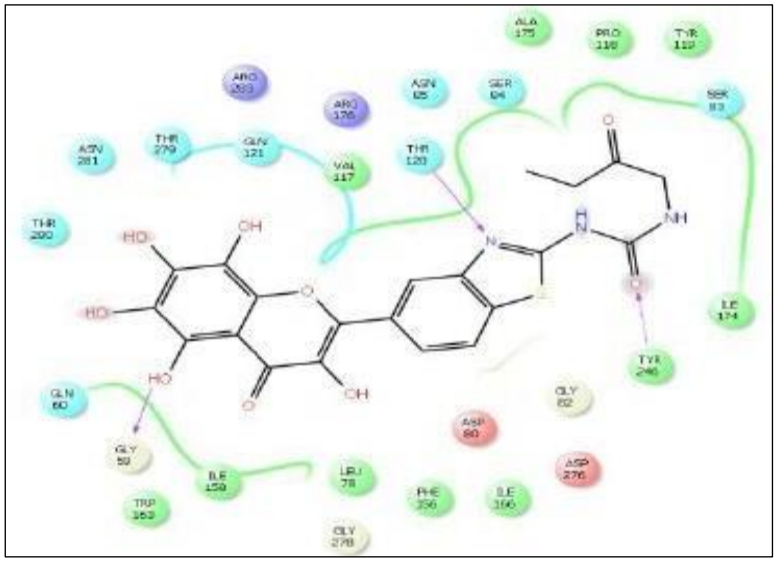

Fig 4.3: Virtual screening

5. VISUALISATION

ϒ Tools for ligand or chemical compound and target molecule optimization include

i) Rasmol
j) VMD
k) Raster 3D
l) Pymol

a) RasMol: -

- A computer application designed for molecular graphics, is used to represent and explore the architecture of biological macromolecules.

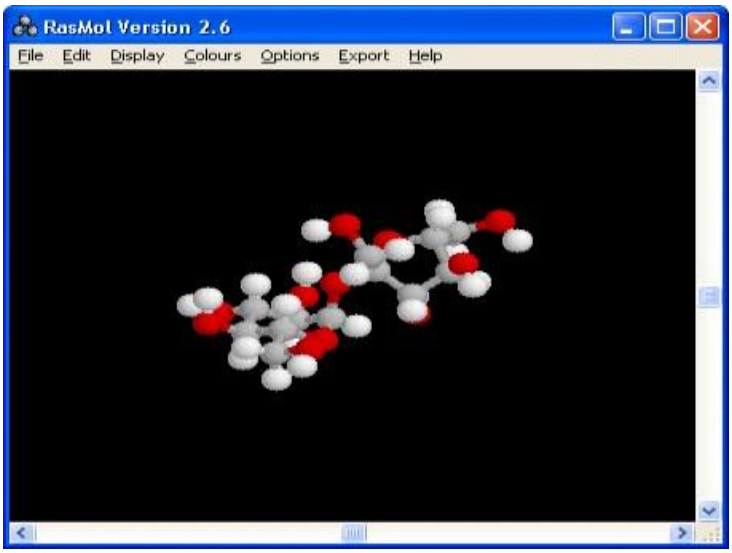

Fig 5.1: Rasmol version 2.6

b) VMD: -

- A computer program for molecular modeling and visualization is called Visual Molecular Dynamics.
- The main purpose of VMD's development is as a tool for viewing and analyzing the outcomes of molecular dynamics simulations.

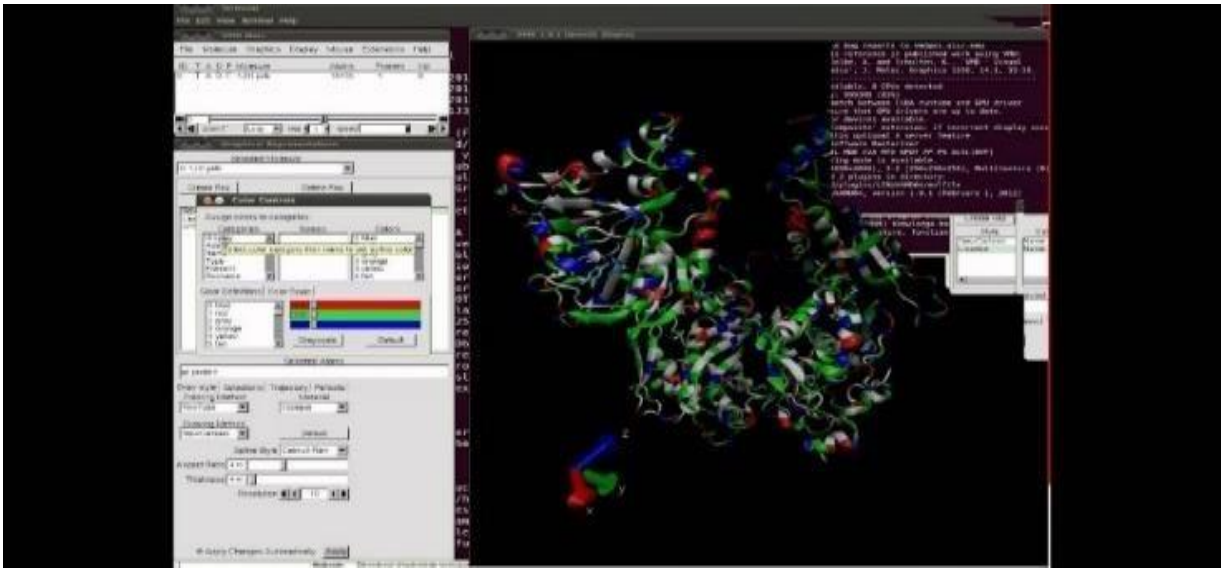

Fig 5.2: Visual Molecular Dynamics

c) Raster 3D: -

- A suite of tools called Raster3D can produce excellent raster images of proteins or other substances.
- Specular highlighting, Phong shading, and shadowing are used to depict spheres, triangles, cylinders, and quadric surfaces in the main programme.

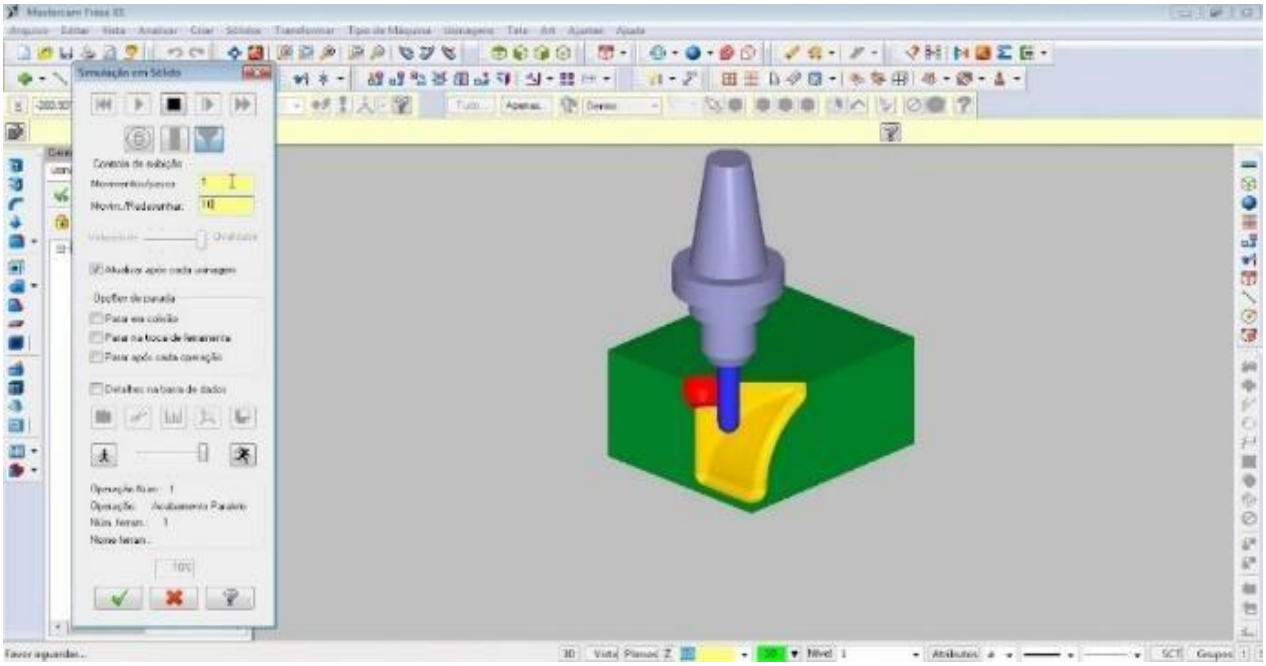

Fig 5.3: Raster 3D

d) PyMOL: -

- PyMOL, a cross-platform molecular graphics programme, has been widely used to visualise proteins, nucleic acids, tiny molecules, electron densities, surfaces, and paths in three dimensions (3D).
- Users can effectively highlight and differentiate several critical structural elements in the targets, notably ideal binding sites for medicinal compounds.

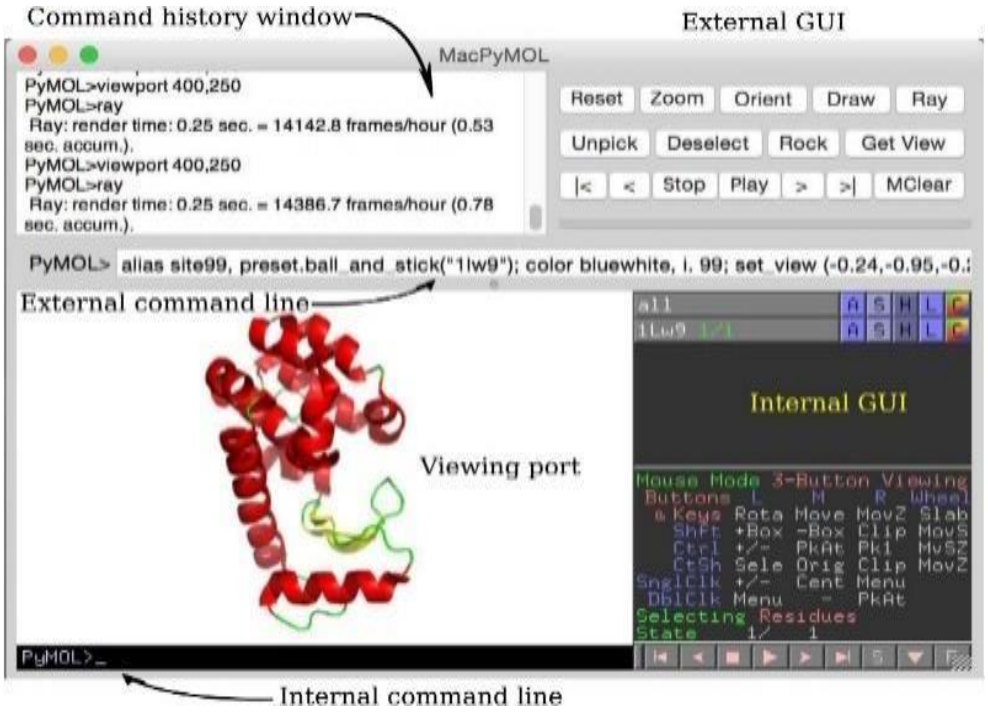

Fig 5.4: Pymol

6. HOMOLOGY AND HOMOLOGY MODELING PROGRAMS

- The majority of pharmacological targets are proteins, it is critical to understand their 3D structures in depth.
- All homology modeling is similar looking for drug analogues.
- It begins with a potential therapeutic molecule.
- There are two programs for homology modeling.
- They are: -

m) **Swiss models**
n) **Modeller**

- The Swiss Model allows you to enter a target sequence and receive an automatically generated comparison model, as long as an empirical structure with >30% sequence identity exists to utilize as a template.
- Modeller is used for 3D protein homology or comparative modelling.

7. PROCEDURE OF CADD

Computer-aided design is target-specific and structure-based, fast and automated, inexpensive, and has a high success rate. The process of facilitating computational approaches and resources utilized in the creation and development of novel therapeutic treatments is known as computer-aided drug design.

CADD has expanded from its typical use of lead finding and optimization to two directions: upstream for target identification and validation, and downstream for preclinical research (ADMET prediction). The first critical stage in the drug discovery process is target identification and validation. However, identifying and validating druggable targets from thousands of candidate macromolecules remains a difficult process. Several technologies for tackling the goals have lately been developed.

The most important techniques for identifying targets are genomic and proteomic methods. Computational methods for drug design are divided into two categories: those that do not presuppose knowledge of the structure of the target macromolecule and those that do. Because the structure of the target macromolecule is unknown, structure-based methods are not yet relevant; in these instances, quantitative structure-activity relationship (QSAR) techniques give the best approach to rational drug design.

A strategy for a structure-based screening campaign, including (i) target selection (ii) library preparation, and (iii) stereochemical quality assessment, ADME/Tox assessment, and computational optimization.

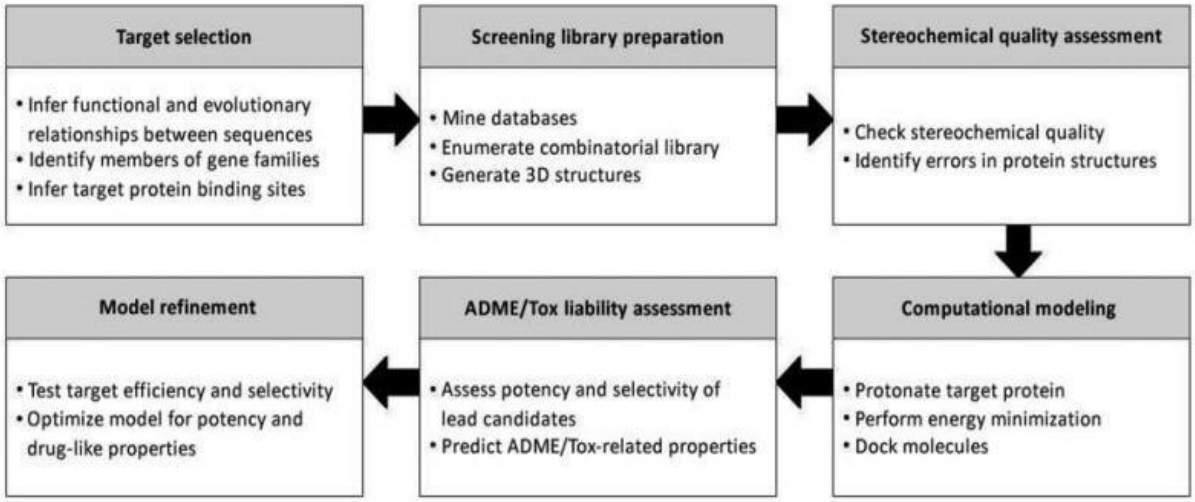

Fig 7.1: Structure-based screening campaign

8. CURRENT ADVANCES IN COMPUTER-AIDED DRUG DESIGN

The effectiveness of a medication discovery and development effort depends on the accessibility of data. Scientific literature and case reports include vast volumes of knowledge about chemical compounds, biological sequences, and related topics. These data are gathered and structurally kept in the databases listed below. Hundreds of biological databases are described each year. Simultaneously, computer techniques are currently being developed to aid in the construction of combinatorial libraries. As a result, computer-aided drug design focuses on these.

Some small molecule databases: -

- PubChem http://pubchem.ncbi.nlm.nih.gov/
- ACD http://www.mdli.com
- ZINC http://zinc.docking.org/
- LIGAND http://www.genome.jp/ligand/
- DrugBank http://www.drugbank.ca/
- ChemDB http://cdb.ics.uci.edu/

9. APPLICATIONS OF COMPUTER-AIDED DRUG DESIGN

- Accuracy
- Less manpower is required
- Database screening
- Chemical & biological information about ligand
- Development of possible drugs for a wide range of diseases
- Potential lead compound
- New microbial targets
- To develop new medications for both established and emerging targets.
- Eliminate the undesirable properties- In-silico filters.

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