TOOLS FOR LIGAND BASED DRUG DISCOVERY

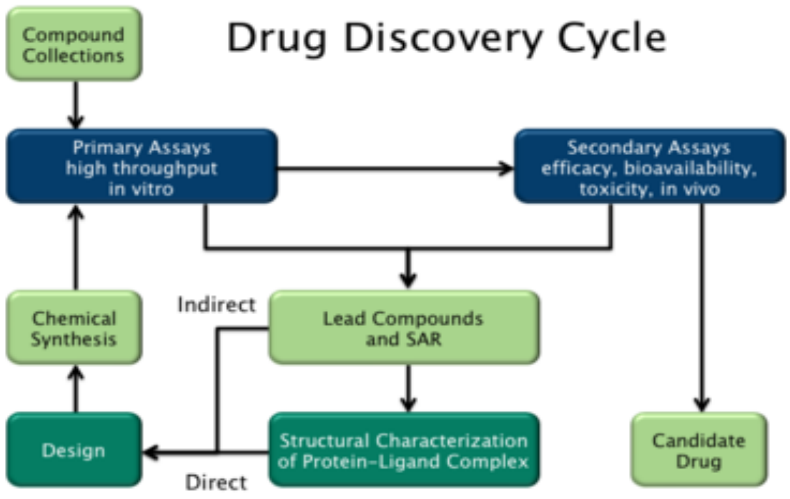
Janvi Gajipara[1] and **John J Georrge**[1*]
[1] *Department of Bioinformatics, Christ College, Rajkot-360 005, Gujarat*
**Corresponding author: janvigaji@gmail.com & johnjgeorrge@gmail.com*

ABSTRACT: The ligand Base drug design also called indirect drug design which relies on knowledge of other molecules that bind to the biological target of interest. These other molecules may be used to derive a Pharmacophore model that defines the minimum necessary structural characteristics a molecule must possess in order to bind to the target. Alternatively, a quantitative structure-activity relationship (QSAR), in which a correlation between calculated properties of molecules and their experimentally determined biological activity may be derived. Target fishing, or target identification, is an important start step in modern drug development, which investigates the mechanism of action of bioactive small molecules by identifying their interacting proteins. Reverse or inverse docking is proving to be a powerful tool for drug repositioning and drug rescue. It involves docking a small-molecule drug/ligand in the potential binding cavities of a set of clinically relevant macromolecular targets. This chapter covers all available tools for the ligand-based drug discovery, which will be beneficial to the researchers who are working on medicinal and/or natural product chemistry.

Keywords: Drug Design, Pharmacophore, QSAR, Reverse Docking

1. INTRODUCTION

Ligand-based drug design or relies on knowledge of other molecules that bind to the biological target of interest. These other molecules may be used to derive a pharmacophore model that defines the minimum necessary structural characteristics a molecule must possess in order to bind to the target. In other words, a model of the biological target may be built based on the knowledge of what binds to it, and this model in turn may be used to design new molecular entities that interact with the target. Alternatively, a quantitative structure-activity relationship (QSAR), in which a correlation between calculated properties of molecules and their experimentally determined biological activity, may be derived. These QSAR relationships in turn may be used to predict the activity of new analogs. Ligand-based drug design uses ligands of the drug target—that is, molecules that bind to the drug target.



Design focuses on the structure of the ligands, for example, by the use of pharmacophore models or by QSAR models. The former model seeks to determine what ligand structures are necessary for target binding. QSAR models, on the other hand, suggest that molecular similarity, through combination molecular descriptors, predicts biological activity of the drug (Cereto-Massagué et al., 2015).

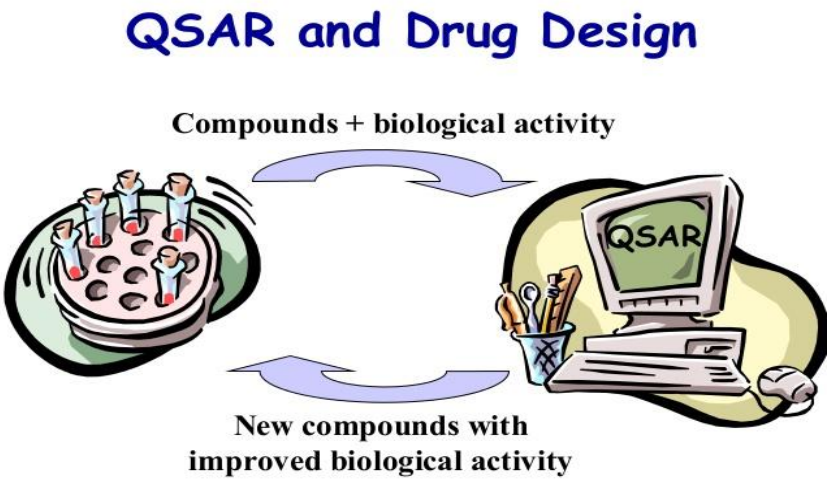
The method available for Ligand based Drug Discovery are QSAR, Pharmacophore, Target Fishing and Reverse Docking. Based on these methods various research works were successfully completed (Chirag N. Patel et al., 2017; Gauravi Trivedi, 2016; John J Georrge, 2015; John J. Georrge, 2016; John J Georrge et al., 2011; John J Georrge et al., 2012; John L, 2012; Joseph et al., 2015; Kotadiya et al., 2015; Nishita NV, 2016; Patel et al., 2017; Rutvi Chovatiya, 2016; Soni et al., 2016; Vyas et al., 2015).

2. QSAR

Quantitative structure–activity relationship models are regression or classification models used in the chemical and biological sciences and engineering. Like other regression models, QSAR regression models relate a set of "predictor" variables (Wolber et al.) to the potency of the response variable (Y), while classification QSAR models relate the predictor variables to a categorical value of the response variable.

The number of compounds required for synthesis in order to place 10 different groups in 4 positions of benzene ring is 10^4.

Solution: synthesize a small number of compounds and from their data derive rules to predict the biological activity of other compounds (Buratto, 2015).



2.1 VEGA platform [https://www.vegahub.eu/portfolio-item/vega-qsar/]

Using the VEGA platform, you can access a series of QSAR models for regulatory purposes, or develop your own model for research purposes. QSAR models can be used to predict the property of a chemical compound, using information obtained from its structure.

2.2 DEMETRA [http://www.demetra-tox.net/]

DEMETRA is an EU-funded project. This project aim has been to develop predictive models and software which give a quantitative prediction of the toxicity of a molecule, in particular molecules of pesticides, candidate pesticides, and their derivatives. The input is the chemical structure of the compound, and the software algorithms use "Quantitative Structure-Activity Relationships" (QSARs). The DEMETRA software tool can be used for toxicity prediction of molecules of pesticides and related compounds. The DEMETRA models are freely available. Five models have been developed to predict toxicity against trout, daphnia, quail and bee. The software is based on the integration of the knowledge acquired in the DEMETRA EU project in a homogeneous manner using the best algorithms obtained as the basis for hybrid combinative models to be used for predictive purposes (Kharkar et al., 2014).

2.3 T.E.S.T [https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test]

Toxicity Estimation Software Tool (T.E.S.T.) will enable users to easily estimate acute toxicity using the above QSAR methodologies.

2.4 OCHEM [https://ochem.eu/home/show.do]

The OCHEM is an online database of experimental measurements integrated with the modeling environment. Submit your experimental data or use the data uploaded by other users to build predictive QSAR models for physical-chemical or biological properties (Lavecchia et al., 2016).

2.5 E-DRAGON [http://www.vcclab.org/lab/edragon/]

E-DRAGON is the electronic remote version of the well-known software DRAGON, which is an application for the calculation of molecular descriptors developed by the Milano Chemometrics and QSAR Research Group of Prof. R. Todeschini. These descriptors can be used to evaluate molecular structure-activity or structure-property relationships, as well as for similarity analysis and high throughput screening of molecule databases.

2.6 SeeSAR [https://www.biosolveit.de/SeeSAR/]

SeeSAR is a software tool for interactive, visual compound prioritization as well as compound evolution. Structure-based design work ideally supports a multi-parameter optimization to maximize the likelihood of success, rather than affinity alone. Having the relevant parameters at hand in combination with real-time visual computer assistance in 3D is one of the strengths of SeeSAR (Lee et al., 2016).

2.7 Dragon [https://chm.kode-solutions.net/products_dragon.php]

Dragon calculates 5,270 molecular descriptors, covering most of the various theoretical approaches. The list of descriptors includes the simplest atom types, functional groups and fragment counts, topological and geometrical descriptors, three-dimensional descriptors, but also several properties estimation (such as logP) and drug-like and lead-like alerts (such as the Lipinski's alert).

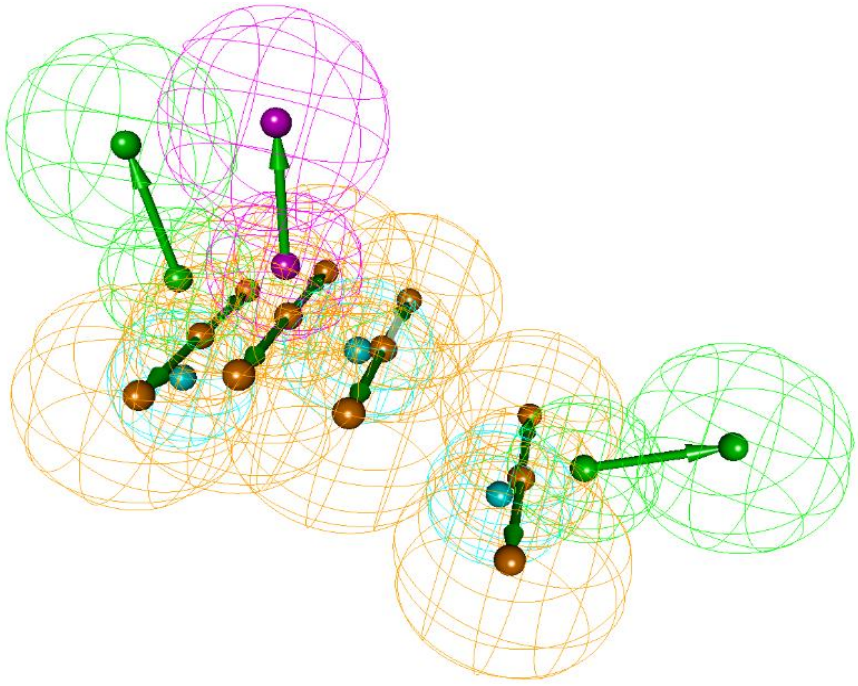
2.8 PaDEL-Descriptor [http://www.yapcwsoft.com/dd/padeldescriptor/]

A software to calculate molecular descriptors and fingerprints. The software currently calculates 1875 descriptors (1444 1D, 2D descriptors and 431 3D descriptors) and 12 types of fingerprints (total 16092 bits). The descriptors and fingerprints are calculated using The Chemistry Development Kit with additional descriptors and fingerprints such as atom type electrotopological state descriptors, Crippen's logP and MR, extended topochemical atom (ETA) descriptors, McGowan volume, molecular linear free energy relation descriptors, ring counts, count of chemical substructures identified by Laggner, and binary fingerprints and count of chemical substructures identified by Klekota and Roth.

3. PHARMACOPHORE

A Pharmacophore is an abstract description of molecular features that are necessary for molecular recognition of a ligand by a biological macromolecule. The IUPAC defines a Pharmacophore to be "an ensemble of steric and electronic features that is necessary to ensure the optimal supramolecular interactions with a specific biological target and to trigger (or block) its biological response". A Pharmacophore model explains how structurally diverse ligands can bind to a common receptor site. Furthermore, Pharmacophore models can be used to identify through de novo design or virtual screening novel ligands that will bind to the same receptor.

In modern computational chemistry, Pharmacophores are used to define the essential features of one or more molecules with the same biological activity. A database of diverse chemical compounds can then be searched for more molecules which share the same features arranged in the same relative orientation.



Pharmacophores are also used as the starting point for developing 3D-QSAR models. Such tools and a related concept of "privileged structures", which are "defined as molecular frameworks which are able of providing useful ligands for more than one type of receptor or enzyme target by judicious structural modifications", aid in drug discovery (Li et al., 2017).

3.1. Pharmer [http://smoothdock.ccbb.pitt.edu/pharmer/]

Pharmer is a pharmacophore search technology that can search millions of chemical structures in seconds. Unlike other technologies, the performance of Pharmer scales with the complexity of the query, not the size of the library being searched. Pharmer powers ZINCPharmer, an online pharmacophore search engine for a multi-conformer library of the ZINC database.

3.2. PharmaGist [http://bioinfo3d.cs.tau.ac.il/pharma/index.html]

Predicting molecular interactions is a major goal in rational drug design. Pharmacophore, which is the spatial arrangement of features that is essential for a molecule to interact with a specific target receptor, is important for achieving this goal. PharmaGist is a freely available web server for pharmacophore detection. The employed method is ligand based. It does not require the structure of the target receptor. Instead, the input is a

set of structures of drug-like molecules that are known to bind to the receptor. We compute candidate pharmacophores by multiple flexible alignments of the input ligands. The main innovation of this approach is that the flexibility of the input ligands is handled explicitly and in deterministic manner within the alignment process. The method is highly efficient, where a typical run with up to 32 drug-like molecules takes seconds to a few minutes on a standard PC. Another important characteristic of the method is the capability of detecting pharmacophores shared by different subsets of input molecules. This capability is a key advantage when the ligands belong to different binding modes or when the input contains outliers.

3.3. Catalyst [http://accelrys.com/products/collaborative-science/biovia-discovery-studio/pharmacophore-and-ligand-based-design.html]

Pharmacophore Modeling and Analysis; 3D database building and searching; Ligand conformer generation and analysis tools; Geometric, descriptor-based querying; Shape-based screening. Distributed by Accelrys as part of Discovery Studio.

3.4. LigandScout [http://www.inteligand.com/ligandscout/]

The LigandScout software suite comprises the most user-friendly molecular design tools available to chemists and modelers worldwide. The platform seamlessly integrates computational technology for designing, filtering, searching and prioritizing molecules for synthesis and biological assessment.

3.5. MOE [https://www.chemcomp.com/MOE-Pharmacophore_Discovery.htm]

MOE contains the industry-leading suite of Pharmacophore discovery applications used for fragment-, ligand- and structure-based design projects. Pharmacophore modeling is a powerful means to generate and use 3D information to search for novel active compounds, particularly when no receptor geometry is available. Pharmacophore methods use a generalized molecular recognition representation and geometric constraints to bypass the structural or chemical class bias of 2D methods (Mori et al., 2015).

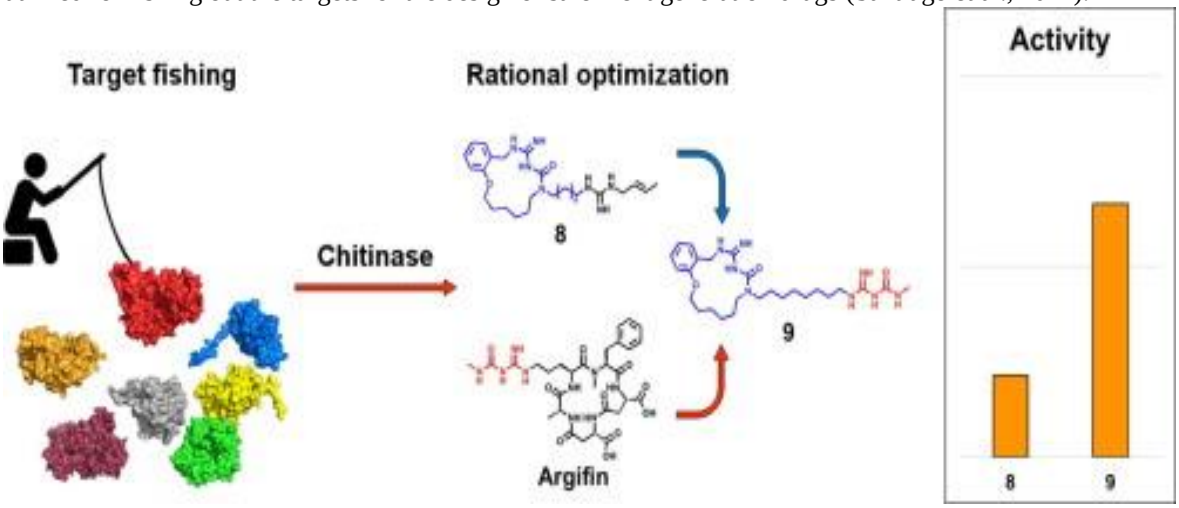
3.6. Phase [https://www.schrodinger.com/phase]

Phase is a complete, user-friendly Pharmacophore modeling solution designed to maximize performance in virtual screening and lead optimization. Fast, accurate, and easy-to-use, Pha**se** includes a novel, scientifically validated common Pharmacophore perception algorithm.

4. TARGET FISHING

Computational methods for Target Fishing (TF), also known as Target Prediction or Polypharmacology Prediction, can be used to discover new targets for small-molecule drugs. This may result in repositioning the drug in a new indication or improving our current understanding of its efficacy and side effects. We can a new benchmark to validate TF methods, which is particularly suited to analyze how predictive performance varies with the query molecule.

Robust target fishing extends multitude benefits to drug research, such as avoiding unwanted side effects from poly pharmacology of small molecules at clinical stages, to reveal the mode-of-actions of a compound and also to repurpose old drugs for new targets. The rule of 'one-size-does-not-fit-all' still holds well in target fishing approaches as well. Therefore, it is important to carefully assemble the available methods and resources such that all levels of biological information, from sequences to structures to pharmacophores, are maximally utilized for fishing out the targets for the design of safer next generation drugs (Santiago et al., 2012).



4.1. ChemMapper [http://lilab.ecust.edu.cn/chemmapper/]

ChemMapper is a free web server for computational drug discovery based on the concept that compounds sharing high 3D similarities may have relatively similar target association profile. ChemMapper integrates nearly 300 000 chemical structures from various sources with pharmacology annotations and over 3 000 000 compounds from commercial and public chemical catalogues. In-house SHAFTS method which combines the strength of molecular shape superposition and chemical feature matching is used in ChemMapper to perform the 3D similarity searching, ranking, and superposition. Taking the user-provided chemical structure as the query, SHAFTS aligns each target compound in the database onto the query and calculates the 3D similarity scores and the top most similar structures are returned. Based on these top most similar structures whose pharmacology annotation is available, a chemical-protein network is constructed and a random walk algorithm is taken to compute the probabilities of the interaction between the query structure and proteins which associated with hit compounds. These potential protein targets ranked by the standard score of the probabilities. ChemMapper can be useful in a variety of polypharmacology, drug repurposing, chemical-target association, virtual screening, and scaffold hopping studies.

4.2. PharmMapper Server [http://lilab.ecust.edu.cn/pharmmapper/index.php]

The current release, i.e. version 2017, is based on the contents of PDB officially released by Jan 1st, 2016. This release applies Cavity1.1 to detect the binding sites on the surface of a given protein structure and rank them according to the corresponding druggability scores. A receptor-based pharmacophore modeling program Pocket 4.0 was then used to extract pharmacophore features within cavities. In this approach, a total of 23236 proteins covering 16159 pharmacophore models which are predicted as druggable binding sites and 52431 pharmacophore models with a pKd value higher than 6.0 are picked out, which is currently the largest collection of this kind. Compared to the last release (v.2010), target pharmacophore models included in this release have increased more than six times, from 7302 to over almost 53000.

4.3. TargetHunter [http://www.cbligand.org/TargetHunter/]

This web portal implements a novel in silico target prediction algorithm, the Targets Associated with its Most Similar Counterparts, by exploring the largest chemogenomical databases, ChEMBL. TargetHunter also features an embedded geography tool, BioassayGeoMap, developed to allow the user easily to search for potential collaborators that can experimentally validate the predicted biological targets or off targets. TargetHunter therefore provides a promising alternative to bridge the knowledge gap between biology and chemistry, and significantly boost the productivity of chemogenomics researchers for in silico drug design and discovery.

4.4. ChemProt [http://potentia.cbs.dtu.dk/ChemProt/]

The ChemProt 2.0 server is a resource of annotated and predicted chemical-protein interactions. The server is a compilation of over 1 100 000 unique chemicals with biological activity for more than 15000 proteins. ChemProt can assist in the in-silico evaluation of small molecules (drugs, environmental chemicals and natural products) with the integration of molecular, cellular and disease-associated proteins complexes.

4.5. SwissTargetPrediction [http://www.swisstargetprediction.ch/]

This website allows you to predict the targets of a small molecule. Using a combination of 2D and 3D similarity measures, it compares the query molecule to a library of 280'000 compounds active on more than 2000 targets of 5 different organisms.

4.6. SuperPred [http://prediction.charite.de/]

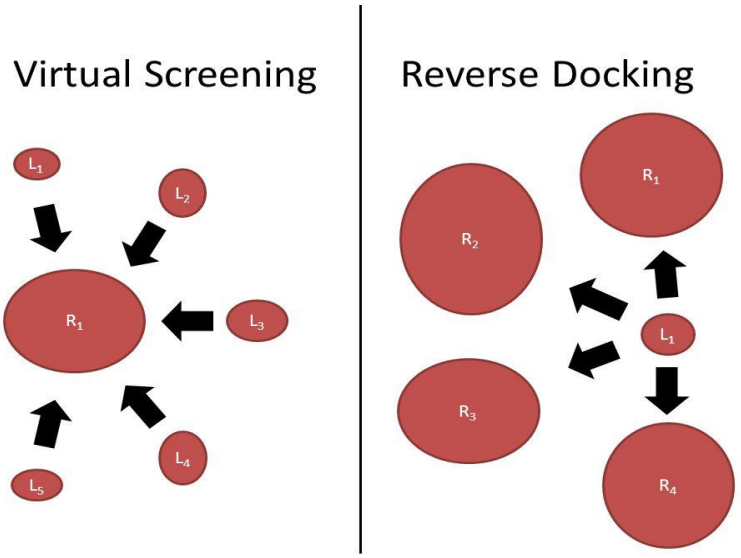
SuperPred, which is a prediction webserver for ATC code and target prediction of compounds. Predicting ATC codes or targets of small molecules and thus gaining information about the compounds offers assistance in the drug development process. The webserver's ATC prediction as well as target prediction is based on a pipeline consisting of 2D, fragment and 3D similarity search.

4.7. PASS [http://www.pharmaexpert.ru/passonline/]

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

5. REVERSE DOCKING

In reverse docking, one tries to find protein targets which can bind to a particular ligand. The necessary components are similar to those of forward docking methods; preparing data sets, searching for ligand poses, and scoring and ranking the complex structures. However, several issues including high computational cost and inter-protein score bias makes reverse docking process rather complex (Wolber et al., 2008).



5.1. INVDOCK [http://bidd.nus.edu.sg/group/softwares/invdock.htm]

A computer method, and its application software INVDOCK, have been developed for computer-automated identification of potential protein and nucleic acid targets of a small molecule. The 3-D structure of the small molecule being studied is input into the programmer, the software automatically searches a protein and nucleic acid 3-D structure database to identify protein, RNA or DNA molecule that the small molecule can bind to. The identified proteins and nucleic acids are considered potential targets of the molecule.

5.2. idTarget [http://idtarget.rcas.sinica.edu.tw]

A web server for identifying biomolecular targets of small chemical molecules with robust scoring functions and a divide-and-conquer docking approach

5.3. AMIDE (Automatic molecular inverse docking engine)

Molecular docking is widely used computational technics that allows studying structure-based interactions complexes between biological objects at the molecular scale. AMIDE was developed, a framework that allows performing inverse virtual screening to carry out a large-scale chemical ligand docking over a large dataset of proteins. Its ability to reproduce experimentally determined structures and binding affinities highlighted that AMIDE allows performing better exploration than existing blind docking methods.

5.4. VTS (Virtual Target Screening)

Virtual Target Screening (VTS)", a set of small drug-like molecules are docked against each structure in the protein library to produce benchmark statistics. This calibration provides a reference for each protein so that hits can be identified for an MOI. VTS can then be used as tool for: drug repositioning, specificity and toxicity testing, identifying potential metabolites, probing protein structures for allosteric sites, and testing focused libraries for selectivity.

5.5. iRAISE (inverse rapid index-based screening engine)

Integrates flexibility of hydrophilic rotatable terminal groups (such as hydroxyl groups) of the active site and the query molecule. iRAISE is an inverse screening tool based on the RApid Index-based Screening Engine (RAISE) technolog.

5.6. ACTP (Autophagic Compound-Target Prediction)

Autophagy (macroautophagy) is well known as an evolutionarily conserved lysosomal degradation process for long-lived proteins and damaged organelles. Recently, accumulating evidence has revealed a series of small-molecule compounds that may activate or inhibit autophagy for therapeutic potential on human diseases. However, targeting autophagy for drug discovery still remains in its infancy. In this study, we developed a webserver called Autophagic Compound-Target Prediction (ACTP) that could predict autophagic targets and relevant pathways for a given compound.

6. CONCLUSION

Here reviewed all four method tools that have been developed so far and discussed about their uses and advantages compared to others. Efforts are needed to validate the results of different prediction methods. In QSAR correlation between calculated properties of molecules and their experimentally determined biological activity may be derived. Target fishing, or target identification, is an important start step in modern drug development, which investigates the mechanism of action of bioactive small molecules by identifying their interacting proteins. Reverse or inverse docking is proving to be a powerful tool for drug repositioning and drug rescue. Examined how servers and tools were built and what algorithms were applied and what methods were used in detail. This review covers all available tools for the ligand-based drug discovery, which will be beneficial to the researchers who are working on medicinal and/or natural product chemistry.

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How to cite this Book Chapter?

APA Style
Janvi Gajipara and John J. Georrge (2018). Tools for ligand based drug discovery. *Proceedings of 10th National Science Symposium on Recent Trends in Science and Technology* (pp. 57-64). ISBN: 9788192952130. Rajkot, Gujarat, India: Christ Publications

MLA Style
Janvi Gajipara and John J. Georrge. "Tools for ligand based drug discovery". *Proceedings of 10th National Science Symposium on Recent Trends in Science and Technology (ISBN: 9788192952130).* Rajkot, Gujarat, India: Christ Publications, 2018. pp. 57-64.

Chicago Style
Janvi Gajipara and John J. Georrge. "Tools for ligand based drug discovery". In *proceedings of 10th National Science Symposium on Recent Trends in Science and Technology (ISBN: 9788192952130*), pp. 57-64. Rajkot, Gujarat, India: Christ Publications, 2018.

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