Review Article

A Comprehensive review of Medicinal Plant Database, Drug Discovery, and Model Organism Databases: Insights into Biomedical Research

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Abstract : In this review, our focus is on biomedical research database that are reported housed mostly by the National institute of Health of the United States .This review presents an overview of three critical domains in biomedical research: medicinal plant databases, drug discovery databases, and model organism databases. By compiling these sources, we aimed to put forth the relevant resources that are key in drug discovery and development. Our focus includes comprehensive searches across multiple databases, including Medicinal Plant Database, Drug Discovery, and Model Organism Databases. Moreover, our investigation on 11 Model organism databases provides valuable insights into drug efficacy, toxicity, and translational research. Medicinal plant databases provide information about classifications, activities, phytochemicals, test targets and structure of phytochemicals in different formats. Drug and drug discovery databases help researchers find and develop new medications by providing organized and accessible information about existing drugs and potential candidates for further study. Brief descriptions of each Database, as well as details including data source, type, study model, availability of access are provided. Furthermore, the entire databases reported here are continuously updating databases according to their user feedbacks and with advancing technologies. Thus, this review highlights how combining updated information from medicinal plants, drug discovery, and model organism databases helps the researchers to make faster progress in medical research and developing treatments.

Keywords: medicinal plant databases; drug discovery databases; model organism databases; biomedical research.

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Introduction

In today's medical world, Databases of medicinal plants that can be used for medicine, Drug discovery databases for finding new drugs, and databases about organisms used in research are really important. These databases serve as critical resources for researchers, healthcare professionals, and pharmaceutical industries alike, offering a wealth of information that drives innovation, enhances efficiency, and improves patient outcomes. Medicinal plant databases provide a comprehensive repository of traditional knowledge and scientific research on the therapeutic properties of plants. In a time when the search for novel drug compounds is more pressing than ever, these databases offer a treasure trove of natural compounds with potential Pharmacological activities. By utilizing the vast diversity of plant species and their bioactive constituents, researchers can identify lead

compounds for drug development, explore alternative therapies, and address unmet medical needs. Similarly, drug discovery databases such as PubChem, ChEMBL, and DrugBank play a pivotal role in accelerating the drug discovery process. With extensive collections of chemical compounds, bioactivity data, and pharmacological information, these databases facilitate the identification of potential drug targets, the screening of compound libraries, and the optimization of lead compounds. Moreover, model organism databases offer invaluable resources for studying human biology, disease mechanisms, and drug responses in vivo. Model organisms such as mice, fruit flies, nematodes, and zebra fish provide tractable systems for genetic manipulation, phenotypic analysis, and preclinical testing. By studying these model systems, researchers can gain insights into the molecular basis of diseases, validate therapeutic targets, and evaluate the efficacy and safety of drug candidates.

This review highlights how combining information from medicinal plants, drug discovery, and model organism databases helps us make faster progress in medical research and developing treatments. Databases discussed in this review are freely accessible.

Medicinal Plant Database

A medicinal plant database is a comprehensive collection of information regarding various plant species known for their therapeutic properties. These databases typically include details such as the botanical classification, geographical distribution, traditional uses, phytochemical composition, pharmacological activities, Different activities (Anti-bacterial,Anti-Fungal,Anti-viral,Anti-Viral,Anti-cancer), 2D and 3D structures of the compounds, Therapeutic uses, and their targets. Some of the Databases are specific for particular Disease.

Medicinal plant database	Plants count	Phytochemicals	Activities/targets/therapeutic use	website link
MPD3 (Medicinal Plants Database for Drug Designing)	1022 different plants	7062	80 Different activites,200+ targets (fungal, viral, bacterial, cancer, insects, snake bites)	https://mpd3.com/
MPDB 2.0 database	More than 500 indigenous medicinal plants of Bangladesh.	24578	Highly focused upon human diseases. Research and clinical industries, for instance in developing nutraceuticals, nutrition products, insecticide	https://www.medicinalplantbd.com/
IMPPAT 2.0: An Enhanced and Expanded Phytochemical Atlas of Indian Medicinal Plants	4010 Indian medicinal plants	17967	•1095 Therapeutic uses. •Number of plant–part–phytochemical associations 189,386 •Number of plant–phytochemical associations 124,995	https://cb.imsc.res.in/imppat
Anti Mtb medicinal plant database	118 native Indian anti-tubercular medicinal plants	3374	Anti-tubercular (anti-TB) activities	https://www.ammpdb.com/

Applications

Medicinal plant databases serve as vital tools for various applications in biomedical research and healthcare. Researchers utilize these databases to identify potential therapeutic compounds, elucidate their pharmacological activities, and explore their traditional uses across different cultures. These databases provide researchers with access to extensive information on the chemical composition, pharmacological activities, and traditional uses of medicinal plants.

Drug Discovery Database

PubChem, ChEMBL, and DrugBank are prominent drug discovery databases that serve as invaluable resources for researchers worldwide. PubChem, maintained by the National Center for Biotechnology Information (NCBI), houses a vast collection of chemical compounds, including information on their biological activities, structures, and associated literature. ChEMBL, curated by the European Bioinformatics Institute (EBI), focuses on bioactivity data for small molecules, providing comprehensive coverage of drug targets, drug-like compounds, and their interactions. DrugBank, a comprehensive pharmacological database, offers detailed information on drug targets, pharmacology, pharmacokinetics, and drug-drug interactions, making it an indispensable tool for drug discovery and development. Together, these databases facilitate the exploration of chemical space, target identification, lead optimization, and drug repurposing efforts, ultimately accelerating the discovery of novel therapeutic agents.

Applications

PubChem, ChEMBL, and DrugBank are essential resources in the field of drug discovery, each offering unique advantages to researchers. PubChem providing information on millions of chemical compounds, including their structures, bioactivities, and references to the scientific literature. ChEMBL focuses on bioactivity data for small molecules, providing detailed information on drug targets, pharmacology, and drug-like compounds, facilitating target identification and lead optimization. DrugBank, a comprehensive pharmacological database, offers wide range of data on drug targets, drug mechanisms, pharmacokinetics, and drug interactions, enabling researchers to explore the properties of approved drugs, investigational agents, and experimental compounds.

Database	Information	Composition	Wedsite link
ChEMBL: a large-scale bioactivity database for drug discovery	Binding, functional and ADMET information for a large number of drug-like bioactive compounds	5.4 million bioactivity measurements for more than 1 million compounds and 5200 protein targets	https://www.ebi.ac.uk/chembldb.
PubChem Substance and Compound databases	Chemical substances and their biological activities	Composition of three inter-linked databases, Substance, Compound and BioAssay. The Substance database contains chemical information, the Compound database stores unique chemical structures. the BioAssay database contains Biological activity data	https://pubchem.ncbi.nlm.nih.gov

		of chemical substances tested in assay	
DrugBank: a comprehensive resource for in silico drug discovery and exploration	Drug (i.e. chemical) data with comprehensive drug target (i.e. protein) information.	Contains >4100 drug entries including >800 FDA approved small molecule and biotech drugs as well as >3200 experimental drugs. Additionally, >14 000 protein or drug target sequences are linked to these drug entries	http://redpoll.pharmacy.ualberta.ca/drugbank/.

Model organism database

Model organisms play a crucial role in scientific research by providing simplified and controllable systems to investigate fundamental biological processes and complex diseases. . By studying model organisms, researchers can explain fundamental principles of genetics, development, physiology, and behavior. In researching human disease, model organisms allow for better understanding the disease process without the added risk of harming an actual human. There are many model organisms; studying model organisms can be informative**.** Understanding the course of a particular disease in humans might take a long time. But a model organism has the ability to rapidly develop a disease and its symptoms. This helps scientists learn and understand the disease in a short period of time. Therefore, model organisms help in examining the cause of newly formed diseases. Overtime, model organisms have become essential tools in clinical research.

Model organism (scientific name)	Common name	Study	Database	Website link
Escherichia coli	Bacteria	Prokaryotic model organism	**EcoCyc**	http://EcoCyc.org
Saccharomyces cerevisiae	Baker's yeast	Model organism for studying eukaryal biology	**Saccharomyces Genome Database**	http://www.yeastgenome.org
Neurospora crassa	Fungus	Model organism for fungal virology	**FungiDB**	http://fungidb.org
Dictyostelium Discoideum	Cellular slime mold	Social amoeba(non-mammalian biomedical model)	**dictyBase**	http://dictybase.org
Caenorhabditis elegans	Nematode worm	Nematodes	**WormBase**	http://www.wormbase.org
Drosophila melanogaster	Fruit Fly	Insects	**FlyBase**	http://flybase.org/
Danio rerio	Zebra Fish	Fish	**Zebrafish Model Organism Database**	http://zfin.org
Mus musculus	Mouse	Mammals	**Mouse Genome Database**	http://www.informatics.jax.org
Rattus norvegicus	Rat	Mammals	**Rat Genome Database**	https://rgd.mcw.edu
Xenopus laevis	African Clawed Frog	Frog	**Xenbase**	www.xenbase.org
Arabidopsis thaliana	Thale cress	Plant	**CressInt, (TAIR)**	http://cressint.cchmc.org http://www.arabidopsis.org.

Applications

Model organisms serve as invaluable tools in various fields of scientific research, including genetics, developmental biology, and pharmacology. These model systems offer several advantages, including genetic tractability, short generation times, and well-characterized genomes, making them ideal for studying gene function, study disease mechanism, drug metabolism, and complex biological phenomena. Model organisms serve as model system in various biomedical research.

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