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Databases on aromatic plants

Bases de datos sobre plantas aromáticas

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Abstract

Essential oils are a mixture of isoprenoid-type organic compounds that have many biological properties and have been widely used in the cosmetic, food, and pharmaceutical industries, among others. That is why there is a lot of information on this broad group of molecules, in fact, there are specialized databases with detailed information on different essential oils from different types of plants. This review aimed to search the existing databases with information on essential oils. The search of the databases was carried out using the keywords databases and essential oils in different search engines. This yielded a variety of specialized databases with detailed information on essential oils and their sources of obtaining them, as well as chemical structures, physicochemical properties, forms of extraction, pharmacological and biological properties, and utility, among others. In conclusion, these essential oil databases have advantages such as the potential to discover new medicines from nature and gather important information for users so that they can easily browse, search, download, and view data on a natural product of interest.

Keywords: Natural products, isoprenoids, database, plants

Resumen

Los aceites esenciales son una mezcla de compuestos orgánicos de tipo isoprenoides que poseen muchas propiedades biológicas, las cuales han sido ampliamente utilizadas en la industria cosmética, de alimentos, farmacéuticas, entre otras. Es por ello por lo que existe bastante información sobre este grupo de moléculas tan amplia, de hecho, hay bases de datos especializadas con información detallada de diferentes aceites esenciales provenientes de distintos tipos de plantas, por lo tanto, el objetivo de esta revisión fue realizar una búsqueda sobre las bases de datos existente con información sobre los aceites esenciales. La búsqueda de las bases de datos se realizó utilizando las palabras claves bases de datos y aceites esenciales en diferentes buscadores. Esta búsqueda arrojó una variedad de bases de datos especializadas con información detallada de aceites esenciales y sus fuentes de obtención, así como estructuras químicas, propiedades fisicoquímicas, formas de extracción, propiedades farmacológicas y biológicas, utilidad, entre otros. En conclusión, estas bases de datos de aceites esenciales tienen ventajas por su potencial para descubrir nuevos medicamentos de la naturaleza y recopilar información importante para los usuarios, de modo que puedan navegar, buscar, descargar y ver fácilmente datos sobre un producto natural de interés.

Palabras clave: Productos naturales, isoprenoides, base de datos, plantas

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Introduction

Aromatic plants are recognized as an important resource worldwide, they have been used for approximately 60,000 years, because they contribute to the development of the economy, to the processing of products in the industry, to marketing, they are an important source of metabolites with pharmacological properties, among others (Tofiño-Rivera et al., 2017). These plants are also known as herbs and spices, they have been used since ancient times as folk medicine and as food preservatives. The best-known aromatic plants, such as oregano, rosemary, sage, anise, and basil, among others, are native to the Mediterranean area. They contain many biologically active compounds, mainly polyphenols, which possess antimicrobial, antioxidant, antiparasitic, antiprotozoal, antifungal, and anti-inflammatory properties. Currently, the demand for these plants and their derivatives has increased because they are natural, eco-friendly, and generally recognized as safe products. Therefore, aromatic plants and their extracts have the potential to become new-generation substances for human and animal nutrition and health (Christaki et al., 2012). Therefore, aromatic plants provide us with a large number of compounds with interesting biological properties, among which we have essential oils, which are an important source of new bioactive molecules, which can replace synthetic chemicals since they are friendly to the environment and are less toxic. Currently, there are more than 20,000 publications in which essential oils are related to some biological activity. This confirms the wide usefulness of essential oils as the main source of bioactive metabolites, which can be used in different areas of our lives (León-Méndez et al., 2019). Several active components of many essential oils are capable of modulating paradoxical responses triggered by different genes and pathways. Consequently, understanding the mechanism of action of bioactive components on the modulation of such paradoxical responses, within a cell or between different cell types, is a prerequisite for developing new therapeutic strategies against many different pathologies. In addition, efforts should be concentrated to investigate the synergistic effects of the bioactive components, which allow a better and more effective response. For an adequate preventive and therapeutic use of essential oils or their active components, the specificity and cytotoxicity must be considered (Saad, Muller and Lobstein, 2013).

On the other hand, plant secondary metabolites and plant-derived extracts represent a valuable reservoir of bioactive compounds: phenols, terpenoids, etc. Consequently, aromatic plants possess a variety of functions with health-related benefits and nutrigenomic implications in gut development and immunity. Currently, there is enormous pressure on the food and feed industry to seek natural, organic, and generally safe substances for use in nutrition. Aromatic plants meet these demands so they can serve as nutraceuticals with many possible commercial applications, such as growth promoters, antimicrobials, immunostimulatory, antioxidants, flavorings, pigments, and preservatives in animals, and alternatives to synthetic substances. The mechanisms of action of these plants are not clear, but the recent development of "omics" techniques provides better knowledge (Christaki et al., 2020). Therefore, this review aims to show the existing databases on aromatic plants and the information available on them.

In a search carried out in the PubMed database using the keywords: "Databases on aromatic plants" it was found that from 2013 to date, 229 articles related to the subject have been published, but few databases of aromatic plants, evidence was found of the use of hallucinatory words to natural products as shown in Figure 1.

Figure 1. Word cloud related to natural products

Information On Databases Of Plants

The search for information or databases on aromatic plants generates very varied and dispersed information among many information sources that present the indomitable task of obtaining complete information, however, international databases have been collecting information in a more controlled manner for decades, so it is possible to find more complete information about aromatic plants (Bartol and Baricevic, 2015). In a search carried out in January 2023 using the keywords aromatic plants and the database in PubMed (https://pubmed.ncbi.nlm.nih.gov/), it was found that there are 229 publications in the last 10 years, however, the part of the publications refers to different biological activities that aromatic plants have, so there is little information compiled in databases on aromatic plants, which demonstrates the need to create new databases on the subject or strengthen existing ones. However, by searching other sources of information, an article was found that reports 120 databases of natural products that have been used in the last 20 years. However, 16% of these are no longer available online, 40% are commercial and their content is not easily accessible. Open resources are usually specialized in a particular type of Natural Products (NP) or lack annotations. For example, the Natural Products Catalogs of the ZINC database are made up of more than 80,000 entries, some of which can be purchased, but apart from their structure and the fact that they are of natural origin, no additional information is provided. Super Natural II is considered the largest among all Natural Products databases, it was available online in 2020, but it seems to be no longer maintained and is mostly made up of purchasable compounds. Another recent database, NPAtlas, is constantly growing and very well annotated, but it focuses solely on microbial NPs. Another important category of NPs, plant-produced compounds, also called phytochemicals, is available in several popular and well-maintained databases, such as NuBBEDB, KnapSack, CMAUP, and TCM@Taiwan. In addition to these relatively large databases, there are a large number of smaller, specialized NP collections, such as FooDB, a user-friendly database that hosts a relatively large number of NPs found in foods. Therefore, there is a need for a generalist NP database, that efficiently aggregates NP information from various sources, improves its annotation, and offers a pleasant user experience (Sorokina and Steinbeck, 2020).

At present there are several databases of aromatic plants, in a work carried out by Maia and Andrade (2009) it describes the creation of a database of aromatic plants of the Amazon, which catalogs general information on 1250 specimens. The database has made it possible to publish the chemical composition of the oils and aromas of more than 350 species, associated with a greater number of chemical types. The essential oils of many species offer optimal conditions for economic exploitation and use in the national and international market for fragrances, cosmetics, and agricultural and domestic pesticides (Maia and Andrade, 2009). Another database is AromaDb (http://bioinfo.cimap.res.in/aromadb/) covers information on plant varieties/chemotypes, essential oils, chemical constituents, GC-MS profile, yield variations due to agromorphological parameters, data trade names, aromatic compounds, fragrance type, and bioactivity details. The database includes 1,321 scent chemical structures, bioactivities of essential oils/scent compounds, 357 fragrance types, 166 commercially used plants, and their 148 high-yielding varieties/chemotypes. It also includes calculated chemoinformatic properties related to identification, physicochemical properties, pharmacokinetics, and toxicological and ecological information. It also comprises interacting human genes that affect various disease-related cell signaling pathways that correlate with aromatherapy use. This database could be a useful resource for plant growers/producers, the flavor/fragrance industry, health professionals, and researchers exploring the potential of essential oils and flavor compounds in developing new formulations against human disease (Kumar et al., 2018).

In India, it was created a comprehensive online database called IMPPAT on the phytochemistry of medicinal plants which will enable computational approaches to drug discovery based on natural products. This database was hand-curated from 1742 Indian medicinal plants, 9596 phytochemicals, and 1124 therapeutic uses spanning 27074 plant phytochemical associations and 11514 plant-therapeutic associations. Notably, the curation effort led to a non-redundant in silico library of 9596 phytochemicals with standard chemical identifiers and structure information. Using cheminformatic approaches, we have computed the physicochemical, ADMET (absorption, distribution, metabolism, excretion, toxicity), and drug-likeliness properties of the IMPPAT phytochemicals. We show that the stereochemical complexity and shape complexity of IMPPAT phytochemicals differs from libraries of commercial compounds or diversity-oriented synthesis compounds while being similar to other libraries of natural products. Within IMPPAT, we have filtered a subset of 960 potential druggable phytochemicals, of which the majority have no significant similarity to existing FDA-approved drugs, thus, rendering them good candidates for prospective drugs. IMPPAT database is openly accessible at: https://cb.imsc.res.in/imppat (Mohanraj et al., 2018). In the case of Latin America, even though we stand out for having a rich and unique biodiversity, which perhaps encompasses a third of global biodiversity, only a few Latin American countries have compiled and characterized the natural products of their region in a database. To the best of our knowledge, research groups in Colombia, Peru, and El Salvador are building composite databases to be released in the future (Gómez-García and Medina-Franco, 2022).

Another example of a database of natural products is COCONUT (https://coconut.naturalproducts.net), this database is free and open to all users and no login is required to access it. Its web interface allows various simple searches (e.g., by molecule name, InChI, InChI key, SMILES, drawn structure, molecular formula), advanced searches by molecular features, along substructure and similarity searches. Users can also download the full data set or search for results in different formats. The database can be queried programmatically via a REST API, making it easy to integrate COCONUT into workflows. The web interface, back-end, and database are implemented as Docker containers, making it easy to port to host other NP sets and deploy on-premises (Sorokina et al., 2021).

Carrying out a search of databases of natural products in general from the year 2013 onwards, 47 databases focused on collecting information related to natural products have been found, however, few are specifically focused on aromatic plants (Table 1).

There are different types of databases, the general ones that contain information on natural and synthetic molecules, and there are the specialized ones that only contain information on natural products, within these we have commercial and Open access. We could identify a total of 92 open-access NP resources across the literature in the last 20 years. The concept of "Open access" encourages and prioritizes free and open online access to academic information, such as data and scientific publications. For a dataset, whether in a database or attached as additional information to an article, it means that anyone can read, download, copy, distribute, print, search for, and within and re-use all or parts of data that

Table 1. Natural Products Databases

Database	Description	References
AromaDb	Database of Medicinal and Aromatic Plant's Aroma Molecules With Phytochemistry and Therapeutic Potentials	Kumar et al., 2018
phytochemdb	a platform for virtual screening and computer-aided drug designing https://phytochemdb.com/.	Mahmud et al., 2022
MPD3	a useful medicinal plants database for drug designing	Mumtaz et al., 2017
Uttarakhand Medicinal Plants Database (UMPDB):	A Platform for Exploring Genomic, Chemical, and Traditional Knowledge	Kumar et al., 2018
OSADHI	An online structural and analytics-based database for herbs of India	Kiewhuo et al., 2023
North East India Medicinal Plants Database (NEI-MPDB)	The present study is an attempt to develop a comprehensive resource of the medicinal plants with a quantitative analysis of the phytochemicals which can enhance knowledge on therapeutic indications and contribute to drug discovery and development	Kiewhuo et al., 2022

MPDB 2.0	A large-scale and integrated medicinal plant database of Bangladesh	Hussain et al., 2021
CDK4	As a phytochemical-based anticancer drug target	Ashraf et al., 2022
NeMedPlant	A database of therapeutic applications and chemical constituents of medicinal plants from the north-east region of India	Meetei et al., 2012
DiaNat-DB	A molecular database of antidiabetic compounds from medicinal plants	Madariaga-Mazón et al., 2021
IMPPAT	A curated database of Indian Medicinal Plants, Phytochemistry and Therapeutics	Mohanraj et al., 2018
IMPPAT 2.0	an enhanced and expanded phytochemical atlas of Indian medicinal plants	Vivek-Ananth et al., 2023
NANPDB	A Resource for Natural Products from Northern African Sources	Ntie-Kang et al., 2017
COCONUT online	Collection of Open Natural Products Database	Sorokina et al., 2021
NP Navigator	A New Look at the Natural Product Chemical Space	Zabolotna et al., 2021
NPASS database update 2023	Quantitative natural product activity and species source database for biomedical research	Zhao et al., 2023
CMAUP	A database of collective molecular activities of useful plants	Zeng et al., 2019
SANCDB	An update on South African natural compounds and their readily available analogs	Diallo et al., 2021
SerpentinaDB	A database of plant-derived molecules of Rauvolfia serpentina	Pathania et al., 2015
MeFSAT	A curated natural product database specific to secondary metabolites of medicinal fungi	Vivek-Ananth et al., 2022
SuperNatural II	A database of natural products	Banerjee et al., 2015
SuperNatural 3.0	A database of natural products and natural product-based derivatives	Gallo et al., 2023
SuperNatural	A searchable database of available natural compounds	Dunkel et al., 2006
ConMedNP	A natural product library from Central African medicinal plants for drug discovery	Ntie-Kang et al., 2014
AfroDb	A Select Highly Potent and Diverse Natural Product Library from African Medicinal Plants	Ntie-Kang et al., 2013
MedPServer	A database for the identification of therapeutic targets and novel leads about natural products	Potshangbam et al., 2018
BioPhytMol	A drug discovery community resource on anti-mycobacterial phytomolecules and plant extracts	Sharma et al., 2014
SANCDB	A South African natural compound database	Hatherley et al., 2015
TM-MC	A database of medicinal materials and chemical compounds in Northeast Asian traditional medicine	Kim et al., 2015
LTM-TCM	A Comprehensive Database for the Linking of Traditional Chinese Medicine with Modern Medicine at Molecular and Phenotypic Levels.	Li et al., 2022

TCMID	Traditional Chinese medicine integrative database for herb molecular mechanism analysis	Xue et al., 2013
YaTCM	Yet another Traditional Chinese Medicine Database for Drug Discovery	Li et al., 2018
ETCM	An Encyclopedia of Traditional Chinese Medicine	Xu et al., 2019
HERB	A high-throughput experiment- and reference-guided database of traditional Chinese medicine	Fang et al., 2021
TCMPG	An integrative database for traditional Chinese medicine plant genomes	Meng et al., 2022
IrGO	Iranian traditional medicine General Ontology and knowledge base	Naghizadeh et al., 2021
CPMCP	A database of Chinese patent medicine and compound prescription	Sun et al., 2022
SymMap	An integrative database of traditional Chinese medicine enhanced by symptom mapping	Wu et al., 2019
TCMSID	A simplified integrated database for drug discovery from traditional Chinese Medicine	Zhang et al., 2022
TCMID 2.0	A comprehensive resource for TCM	Huang et al., 2017
TCMIO	A Comprehensive Database of Traditional Chinese Medicine on Immuno-Oncology	Liu et al., 2020
Plant Metabolite Databases	From Herbal Medicines to Modern Drug Discovery	Nguyen-Vo et al., 2029
UNaProd	A Universal Natural Product Database for Materia Medica of Iranian Traditional Medicine	Naghizadeh et al., 2020
SistematX	An Online Web-Based Cheminformatics Tool for Data Management of Secondary Metabolites	Scotti et al., 2018
VIETHERB	A Database for Vietnamese Herbal Species	Nguyen-Vo et al., 2029
GreenMolBD	Nature Derived Bioactive Molecules' Database	Hosen et al., 2022
ETM-DB	Integrated Ethiopian traditional herbal medicine and phytochemicals database	Fathifar et al., 2019

are contained in it (Sorokina and Steinbeck, 2020). Databases on natural products have advantages such as the potential to discover new medicines from nature and collect important information for users so that they can easily browse search, download, and view data on a natural product of interest (Fathifar et al., 2023).

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