

MalagasyplantsDB: a database of essential oils from malagasy plants

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ABSTRACT

Numerous studies have been conducted on plants with essential oils and on their compositions and activities. However, to our knowledge, there is currently no essential oils database of malagasy plants that can simultaneously provide comprehensive information on essential oils, plants and chemical compounds. MalagasyplantsDB is a database of essential oils from Madagascar containing profiles experimentally recorded in several scientific publications. The database contains botanical information for each plant species, including scientific name, common name, taxonomy and ethnobotany. For each record in essential oil profiles, experimental conditions, chemical compound, physicochemical and organoleptic characteristics are provided. For each compound, the chemical identity of the compound, nomenclature possibilities and stereoisomers are provided. Data was compiled from existing literature: peer reviewed journals, doctoral thesis, books and web-sources. MalagasyplantsDB is available on www.malagasyplantsdb.polytechnique.mg. The database includes a total of 109,875 records with 298 essential oil profiles, 336 chemical compounds and 6,125 species or varieties of plant data. Information was collected from 3603 references.

Keyword: - Botany, Chemical compound, Database, Essential oil, Ethnobotany, Madagascar.

1. INTRODUCTION

Madagascar has one of the largest and most important biodiversity sites in the world. Due to its evolution in relative isolation in 400 million years, Madagascar is an exceptional refuge for plants and animal species not found anywhere else. [1], [2]

The relief of Madagascar is characterized by its asymmetry from west to east. On the one hand, the island's center involves in the highlands and a chain of valleys surrounded and separated by mountain ranges with an average altitude of 1300 m above sea level. On the other hand, the coasts are a belt of extensive plain and have their own specific fauna and flora. The climate is subsequently asymmetric and the vegetation of Madagascar extends over the entire island in a non-homogeneous way [3]. It has long attracted the interest of botanists and still captures the imagination of naturalists worldwide.

If the history of botany and the inventory of flora in Madagascar began in 1658, with the publication of Flacourt [4], the first inventory of aromatic plants in Madagascar was carried out much later in 1921, by Gattefossé [5]. Various aromatic plants of economic value were introduced in Madagascar before and during the colonial period, mainly cloves, ylang-ylang, patchouli, vetiver and niaouli [6]. Investigation of endemic aromatic plants started later and the origin and bio-ecological distribution of Madagascar's aromatic plants were described in 1996 [7]. Since then, numerous independent studies have been conducted on plants with essential oils and on their compositions and activities [8], [9], [10], [11]. Several authors reported many factors influencing the chemical variability of essential oils [12], [13], [14]. However, to our knowledge, there is currently no essential oils database of malagasy plants that can simultaneously provide comprehensive information on essential oils, plants and chemical compounds.

Malagasyplantsdb is a database of essential oils from Madagascar containing profiles experimentally recorded in several scientific publications. The main interest of the database is the provision of data. The database organizes all the information itself and could link them together. The objective is to create a practical tool to help researchers, students and industrialists gain a better understanding of essential oils from Malagasy plants.

2. METHODOLOGY

MalagasyplantsDB contains key information for each species, each plant and each chemical composition. The database contains botanical information for each plant species, including scientific name, common name, taxonomy and ethnobotany. For each record in essential oil profiles, experimental conditions, chemical compound, physicochemical and organoleptic characteristics are provided. For each compound, the chemical identity of the compound is provided (CAS number, formula, chromatogram and mass spectra, molecular weight, IUPAC, molecular structure), nomenclature possibilities (trivial names, IUPAC names, names in different languages, trade names...) and stereoisomers if necessary. Complete literature citations are available for every single record.

2.1 Data Collection

The database is divided into three closely related sections: a section on plants, on essential oil profiles and on chemical compounds.

- Essential oil profiles section

Essential oil profiles were compiled from existing literature: peer reviewed journals and doctoral thesis. From each record, the identity of the plant is extracted, the part of the source plant, the time and place of collection, the method of identification and the quantity of each chemical compound. In addition, if an essential oil has, for example, 10 different chemical compounds, we process this data in ten independent records.

- Plant section

Information on plants such as taxonomy, common name, photos and ethnobotanical data were compiled from 49 books and a few public and free web-resources Tropicos (www.tropicos.org/) ITIS (<http://www.itis.gov/>), catalogue de Madagascar (<http://www.efloras.org/>).

- Chemical compound section

For each compound in the database, CAS number, IUPAC name, chemical formula, chemical classifications, stereoisomers, synonyms, retention indices and mass spectra are collected. Information on each chemical compound was collected from web-resources : the NIST (<http://webbook.nist.gov/>), PubChem (<https://pubchem.ncbi.nlm.nih.gov>); Common Chemistry (<http://www.commonchemistry.org>); MassBank (www.massbank.jp). For the retention indices of the compounds, each recorded item of data is provided with citations from the literature. The retention indices were collected from 3485 bibliographic references. These references can be consulted in the database. Mass spectra were collected in Adams [15].

2.2 Database development

MalagasyplantsDB is accessible on www.malagasyplantsdb.polytechnique.mg. Malagasyplantsdb database was prepared using MySQL and the web database was created PHP.

The database at the chemical compound section is divided into 5 tables: identity, other names stereoisomers, retention indices and references. The database in the plant section is divided into 4 tables: plant, common names, ethnobotany and botanical description. The essential oil profiles section links these two ones by plant names and chemical compounds.

3. RESULTS AND DISCUSSION

3.1 Database content

To date, the database contains a total of 109,875 records from around 50 years of published essential oil profile reports and a century of published ethnobotanical and retention index data. These records come from 3603 references.

- Essential oil profile section

The database contains 298 essential oil profiles which include 59 species or varieties spread over 20 families, representing about 70% of the total aromatic species declared by the Ministry of the Environment [16]. These profiles come from 69 references.

The essential oil profiles of *Cinnamosma fragrans* represent the largest number of records, followed by those of *Cedrelopsis grevei* (31 and 30 profiles respectively).

Essential oils have been extracted from distinct aerial or underground plant structures such as leaves, roots, rhizomes, seeds, bark, flowers or any combination of these or even the entire plant. The plant material used for the extraction is likely to be fresh, or dried.

- Chemical compounds section

The content of the database of chemical compounds is shown in table 1

Table -1: Content of chemical compounds section

Table	Records
Chemical compounds	336
Other names	3024
Retention indices	98116
Stereoisomers	1008

The compounds in the base are divided into 18 chemical class categories such as: acids, aldehydes, monoterpene ketones, sesquiterpene and diterpene ketones, esters, lactones, monoterpenes, monoterpenols, oxides, phenols, sesquiterpenes, sesquiterpenols ...

- Plants section

Data collection recorded 6125 species or varieties grouped in 181 distinct taxonomic families. This figure represents around 45% of plants in all of Madagascar which is estimated at 14,000. [17]

The vernacular names of plants in each region and ethnic group are listed in the database, so that users can search by vernacular names. An average of 3 vernacular names for each species was identified, i.e., a total of 19,453 vernacular names recorded.

3.2 Geographical distribution of aromatic plants in Madagascar

We estimated the geographic distribution of aromatic plants in Madagascar. The locations of collection are represented in the figure 1 by red dots. The figure shows that the origin of plants is mainly concentrated in the centre and the eastern part of Madagascar. This distribution differs somewhat from the distribution of the industrial essential oil sector in eastern and northwest part of Madagascar. Madagascar produced essential oil for the first-time on the east coast. The aromatic species used was for the production of essential oils which were highly demanded in the international market. Northwest is also a region rich in species used to extract essential oils [18]. However, this region is slightly represented in the database for only 4 records with 2 species.

No published data on essential oils has been identified in the Midwest of Madagascar (Melaky, Menabe and Bongolava regions), in the Sava and Sofia regions in the North, as well as in the southern part (Anosy and Androy regions). This could be explained by the fact that these areas are difficult to access by road



Fig -1: Geographical distribution of aromatic plants

3.3 Taxonomic distributions of essential oil plants

We evaluated the taxonomic distributions of essential oil plants in general and by yield (Chart-1). The most represented families in the database are: Asteraceae, Lauraceae, Canellaceae and Rutaceae. Considering the yield, the plants with high volatile compound content represented in the database mainly belongs to the Canellaceae and Lauraceae families.

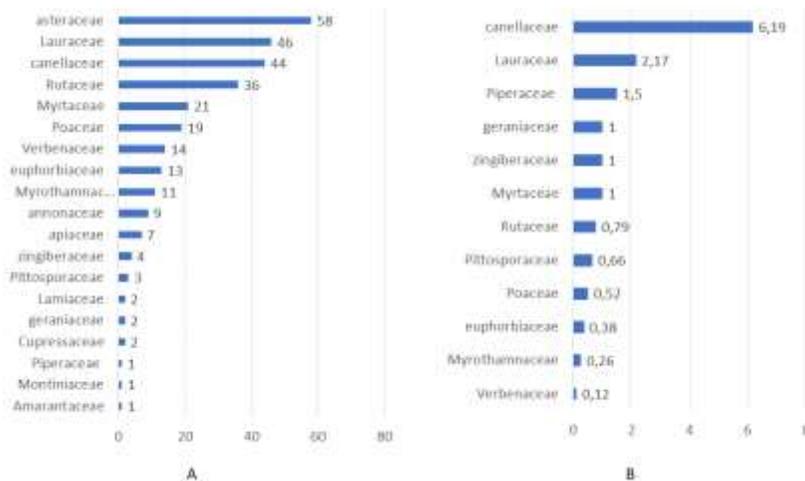


Chart -1: Taxonomic distribution of the aromatic plants in the database in general (A) and by yield (B) work.

3.4 Influence of ecological factors and experimental conditions on the composition of essential oils

Several studies have been conducted to compare the profiles of essential oils under different experimental conditions. The database provides information on environmental factors and experimental conditions associated with essential oil profiles. These factors can be considered individually or in combination with others. Analysis of the database identified 168 records with 8 factors that vary the profiles of essential oils. The chart-2 shows the different types of experimental conditions and their corresponding number of records.

The first variability factor most represented in the database is the geographical distribution with 55 records. The main data in this section include the analysis of the essential oil composition of a plant species across different regions and altitudes. Many studies suggested that the variation in essential oil profiles depends on the variation of ecological factors, such as habitat type, their abundance, and abiotic and biotic factors [19]. In the database, we have the example of *Myrothamnus moschatus* to illustrate. The same species has been found to have different compositions in 5 different regions [20]. In the same way, *Tagetes minuta* shows a variability of its chemical compounds depending on the altitude of the source plant. Plants with a higher rate of *Tagetes* derivatives are located in the Highlands [21].

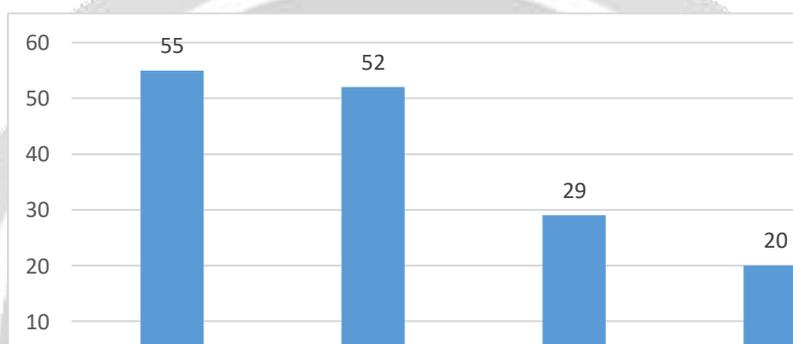


Chart-2 : The different types of experimental conditions and their corresponding number of records

In the database, 52 records show chemotypic variations. The most relevant is chemotypes for *Ravensara aromatica* with seven chemotypes: Estragole, methychavicol, methyleugenol, α -terpinene - limonene, 1,8-cineole, 1,8-cineole - sabinene. [22], [23], [24], [25],

The third factor of variability is the influence of extraction conditions. The main data in this section include: type of extraction, extraction time and extraction fractions. The chemical composition of the product obtained by hydrodistillation differed from the chemical composition of product obtained by steam distillation and both differ from the chemical composition of the mixture initially present in the secretory organs of the plant. Water, acidity and temperature could induce ester hydrolysis, rearrangements, isomerisations, racemizations, oxidations etc. The proportion of sensitive compounds such as linalool, 1,8-cineol, 4-terpineol vary more or less in accordance with the type of extraction [26], [27]. A case in point is the considerable variations from the composition of the essential oil of *Croton kimosorum* obtained by hydrodistillation to the essential oil obtained by steam distillation [28].

Over different collection periods, the plant evolve in different phases. The proportion of the different constituents of an essential oil can vary throughout development. The climate could also be a factor that changes from period to period. To illustrate, the database shows that the chemical profile of *Helichrysum faradifani* varies from season to season. For example, in two different periods, the amount of α -Fenchene varies from 27.3% to 13.1% and the β -caryophyllene from 5.4% to 27.2% [29].

The species phenotype was also reported in the database as a factor of variability in the chemical composition of essential oils with 9 records. For *Lantana camara* for example, two distinct chemotypes was observed in two different phenotypes [14].

3.5 Variability of terpenoids in essential oil plants in Madagascar

Vranovà et al in 2013 suggested that the 2C-Methyl-D-erythritol 4-phosphate (MEP) pathway is preferred in green tissues as compared to mevalonic acid (MVA) pathway in *Arabidopsis thaliana* which has been subjected to a particular circadian rhythm by increasing the time of exposure to light [30]. In theory, the biosynthesis of monoterpenes and diterpenes is occurring in plastid where the MEP pathway is operated, and the biosynthesis of sesquiterpenes occurs in the cytosol through classical MVA pathway [31]. Sangita Kumari et al in 2014, tested this

hypothesis and suggested that the green parts of plants show relatively greater amounts of hemi, mono and diterpenes. The non-green plant parts release higher amounts of sesquiterpenes.

With MalagasyplantsDB, we compared the amount of monoterpene, diterpene and sesquiterpene in green parts of plants and in underground parts and non-green plant parts. The chart-3 shows the proportions of these three chemical classes in each part of the plant with the corresponding data records. The green parts (which contain plastids): leaves, flowers, fruits and aerial parts have a higher percentage of monoterpenes than sesquiterpenes. The roots and bark contain more sesquiterpenes. The results show that diterpene are less abundant than the mono- and sesquiterpenes, reflecting the fact that diterpenes are generally not volatile in nature.

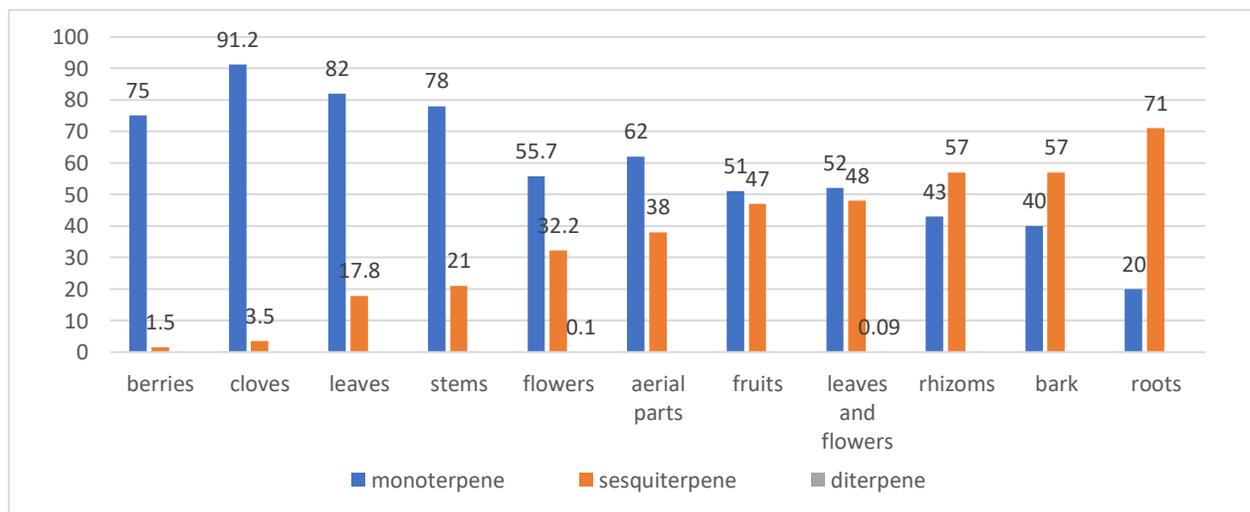


Chart-3: The amount of chemical family in each part of the plant source

3.6 The correlation between biological activities and terpene constituents

We tested from the database whether the composition of essential oils with the same virtues would have similarities. For this, we have exploited the traditional uses and aromatic uses of essential oils in combination with their compositions.

We took the example of "anti-inflammatory". The database provides eight plants and analysis showed mainly three compounds: β -caryophyllene, 1,8-cineole and α -pinene.

β -caryophyllene is the common point of 7 plants traditionally recognized as anti-inflammatory: *Cedrelopsis grevei*, *Helichrysum cordifolium*, *Eucalyptus citriodora*, *Helichrysum gymnocephalum*, *Lantana camara* and *Pelargonium roseum*. Numerous studies suggested the anti-inflammatory activity of β -caryophyllene. It has been tested in vitro on human neuroblastoma cells, its anti-inflammatory activity was very high [32]. β -caryophyllene showed to be a potent nonsteroidal anti-inflammatory agent when tested in vivo [33].

1,8-cineole was present in *Lantana camara*, *Eucalyptus citriodora*, *Psiadia altissima*, *Helichrysum gymnocephalum* and *Pelargonium roseum*. The 1,8-cineole was shown in some studies to be a potential anti-inflammatory in vivo and in vitro model [34], [35].

α -pinene occurred in *Cedrelopsis grevei*, *Eucalyptus citriodora*, *Helichrysum gymnocephalum*, *Lantana camara*, *Pelargonium roseum* and *Psiadia altissima*. α -pinene was reported to have anti-inflammatory activities [36].

We took another example: anxiety. The base provided 8 plants: *Cinnamosma fragrans*, *Cedrelopsis grevei*, *Cinnamomum camphora*, *Cinnamosma fragrans*, *Cymbopogon martini*, *Pelargonium roseum*, *Ravensara aromatica* and *Zingiber officinale*. Among the most important similarities in the composition of these plants, we highlight the following: Linalool, methylchavicol and sabinene.

Several studies support the anxiolytic activity of Linalool. In vivo tests showed that linalool and essential oils rich in this compound can fight anxiety states. [37], [38].

To our knowledge, there are no reports of anxiolytic activities of methyl chavicol. However, we found studies reporting the anxiolytic effects of essential oil of *Ocimum basilicum* that contains a considerable amount of methylchavicol (42.8%) (61). This compound may work on its own or in synergy with others to treat anxiety.

Sabinene. Although the level of sabinene in these plants is average (6 to 14%) This compound represents the highest incidence in the responses (with 75 records for the search for "anxiety"). *Acantholippia deserticola* essential oil has been reported to include Sabinene among its main constituents and exhibit antidepressant and anxiolytic activities. From these examples, it would be possible to predict the activity of the oil by knowing the molecules.

4- CONCLUSION AND FUTURE DEVELOPMENT

The database includes a total of 109,875 records with 298 essential oil profiles, 336 chemical compounds and 6,125 species or varieties of plant data. Information was collected from 3603 references.

The development of MalagasyplantsDB compilations between several studies and several factors that would be useful for scientific and all users wishing to have scientifically rigorous data concerning essential oils in Madagascar.

We plan to expand the data by regularly updating it from upcoming reports. In plant section, common names and ethnobotany are complete for all the 6125 species and data on botanical description are expected to be completed in the near future. As these 6215 species are not all aromatic plants, it will be interesting to develop the extension of the database on chemical compounds of non-volatile extracts. We hope to integrate tables for biological and pharmacological activities for essential oils and extracts. We are also working on a plan to integrate data from analysis tools using theoretical approaches to the graph to provide better insight into user-specific research.

It is a research axis to be exploited in order to link botany, ethnobotany, chemistry and biology, which are in constant dialogue to advance knowledge.

5. ACKNOWLEDGEMENT

Authors thank the Ecole Supérieure Polytechnique d'Antananarivo for hosting MalagasyplantsDB as a subdomain in the website www.polytechnique.mg

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