EssoilDB: A Semantic Knowledge base for Synthetic Phytochemistry

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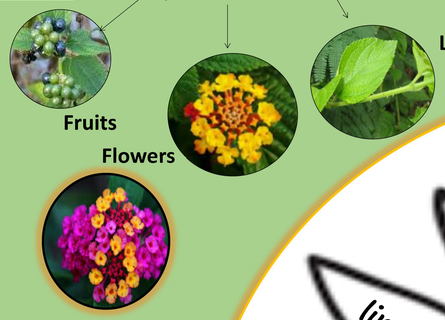
EssOilDB:
The EssOilDB (the ESSential OIL DataBase) is an organized collection of plant volatile emissions, containing experimental records of essential oil composition data, from published reports.

Importance:
Context based scientific research, through a multitude of queries on volatile profiles of native, invasive, normal or stressed plants, across taxonomic clades, geographical locations and several other biotic and abiotic influences.

plant {Records: ca 1800} → **plantpart** → **profile**

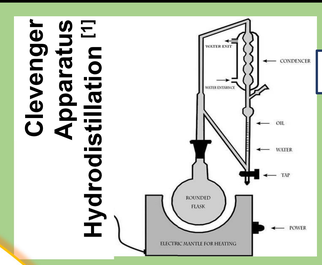
Most commonly used parts of Lantana



profile
Record of the experimental conditions and metadata.

extraction

Clevenger Apparatus Hydrodistillation [1]



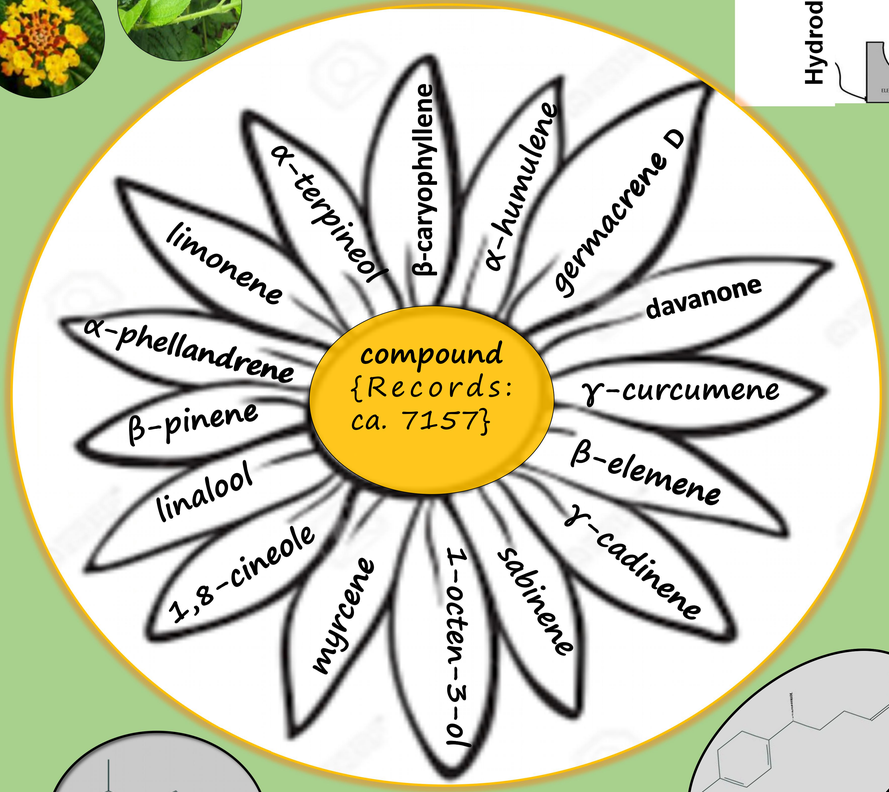
Lantana Essential Oil [4]

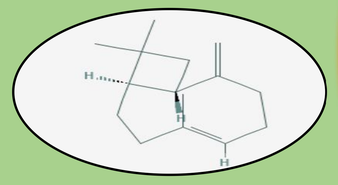
Benefits:
- Potential preventive and therapeutic agents in pharmacology.
- In aroma-therapy, for transdermal delivery of medicines.

analyticaldata

GC/MS Instrument – Agilent Technologies [3]

profiledata
This is the chemical data associated with a profile

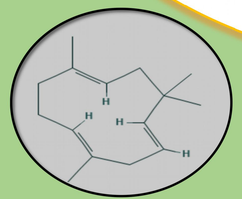




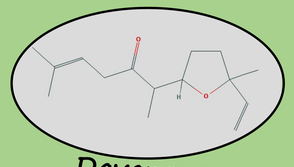
β-caryophyllene

Compound	RI[a]	Leaf oil
eugenol	1160	-
δ-elemene	1340	0.6
β-elemene	1393	1.1
β-caryophyllene	1425	16.2
β-gurjunene	1434	0.3
α-humulene	1456	2.0
germacrene D	1484	28.6
bicyclogermacrene	1489	14.7
germacrene A	1505	0.3
γ-cadinene	1515	0.3
cubebol	1517	0.2
δ-cadinene	1526	1.2
α-cadinene	1540	0.2
elemol	1553	0.3
germacrene B	1560	1.1
(E)-nerolidol	1567	-
germacrene D-4-ol	1579	19.9

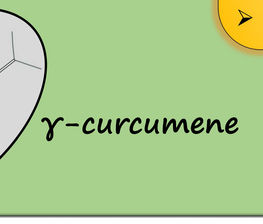
location	
Madagascar	Brazil
Sweden (Goteborg)	Cameroon
India	Cuba
Iran	Egypt
Nigeria	Ethiopia
South China	South Benin
Algeria	



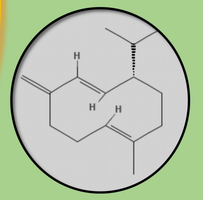
α-humulene



Davanone



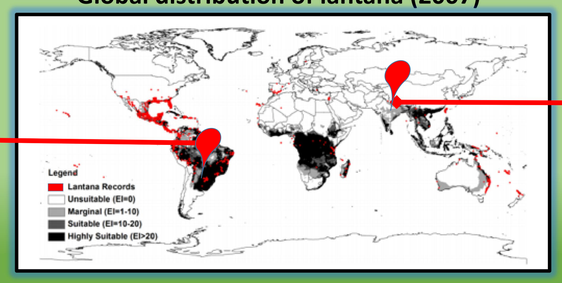
γ-curcumene



germacrene D

Inferences:
- The most prominent essential oil produced by a particular species
- The part of the plant which yields maximum amount of the desired compound
- The location at which a particular species produes maximum amount of terpenes
- Seasonal changes in the production of essential oils

Global distribution of lantana (2007)



Essential Oil Composition of Two *Lantana* Species from Mountain Forests of Pernambuco (Northeast of Brazil)

José C. S. de Oliveira , Ilzenayde A. Neves , Claudio A. G. da Camara & Manfred O. E. Schwartz

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Chemical Composition of the Leaf Oil of *Lantana camara*

Virendra S. Rana , D. Prasad & M. Amaro Blazquez

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To link to this article: https://doi.org/10.1080/10412905.2005.9698874

Table I. Chemical constituents of *Lantana camara* leaf oil

Compound	RI	Area (%)	Compound	RI	Area (%)
Monoterpene hydrocarbons			borneol	789	0.1
α-pinene	315	0.5	terpinen-4-ol	819	0.3
sabinene	378	2.2	α-terpineol	851	0.6
β-pinene	385	0.7	verbenone	893	0.1
myrcene	413	1.2			
α-phellandrene	435	0.6	**Sesquiterpene hydrocarbons**		
p-cymene	470	0.1	α-copaene	1338	0.4
limonene	477	0.6	β-elemene	1376	2.8
(Z)-β-ocimene	497	0.4	β-caryophyllene	1446	23.3
(E)-β-ocimene	517	0.4	α-humulene	1529	11.5
γ-terpinene	548	0.1	γ-curcumene	1596	6.3
terpinolene	605	0.1	germacrene D	1598	10.9
			γ-cadinene	1703	2.3
Oxygenated monoterpenes					
1-octen-3-ol	386	1.3	**Oxygenated sesquiterpenes**		
3-octanol	517	0.3	davanone	-	7.3
1,8-cineole	483	0.7	caryophyllene oxide	1864	0.3
linalool	644	0.7	T-cadinol	1974	0.3
camphor	732	0.1			

Conclusions:
Creation of EssOilDB is an attempt to provide a systematic compilation of essential oil profiles along with the details of their sources for the benefit of not only scientific community but also for the layman, entrepreneurs and farmers in exploring volatiles and their properties. As evident from the benchmarking analysis presented here, EssOilDB is the first and only database that enables a rigorous scientific assessment of plant essential oils in context of their surroundings and in a comparative manner.

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- The outline of the flower was taken from http://clipartmag.com/images/sunflower-black-and-white-clipart-11.jpg . All the other images are taken from Wikimedia