Original Research

Chemical comparison between essential oil, hydrolate and spagyric quintessence.

Nathan Barros da Rocha [1,2], Bernardo Starling Albuquerque Penido Silva [3], Ellen Tanus Rangel [4], Daniel Luiz Reis Simas [2, 5]

[1] Universidade Federal do Rio de Janeiro – IPPN/CCS/UFRJ, Rio de Janeiro, Rio de Janeiro, Brazil.
[2] Bio Assets Biotecnologia – CIETEC/USP, São Paulo, São Paulo, Brazil.
[3] Hermes Esparigia, Brumadinho, Minas Gerais, Brazil.
[4] Universidade Federal de Goiás - Laboratório de Bioprodutos/FF/UFG, Goiânia, Brazil.
[5] Universidade do Estado de São Paulo – LQPN/IQ/USP, São Paulo, São Paulo, Brazil.

* Correspondence: danielsimas16@gmail.com

Abstract: Essential oils, hydrolates, and spagyric quintessences have been gaining prominence in healthcare. This work investigates the volatile chemical composition of these three plant-based products derived from geranium (*Pelargonium graveolens*), erva-baleeira (*Varronia curassavica*), and dentata lavender (*Lavandula dentata*), comparing them to support their rational use. The compositions of essential oils, hydrolates, and spagyric quintessences were divided into three classes: oxygenated terpenes (O), monoterpene hydrocarbons (M), and sesquiterpene hydrocarbons (S). The products showed distinct compositions and proportions within these classes; the spagyric quintessence showed an intermediate volatile composition between the essential oil and hydrolate. On the other hand, the essential oil and hydrolate showed contrasting compositions. This difference indicates that the use of each product may not be directly correlated.

Keywords: chemical composition, therapeutic applications, production processes, aromatic products.

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1. Introduction

Natural products have been used for curative purposes throughout human history. Plants are one of the most widely used natural products for treating or attenuating diseases, and they are attested in traditional medicine practices (1). With the development of modern medicine and pharmaceutical chemistry, synthetic and semi-synthetic drugs became central to conventional therapeutics, although plant-derived products continued to play an important role in many traditional and complementary medicine systems. In the last years integrative practices and traditional medicines have been gaining space in healthcare. Beyond the use of medicinal plant's extracts, essential oils, hydrolate and spagyric quintessence are used too in alternative practices (2).

Essential oils are concentrated plant extracts composed of volatile compounds, obtained primarily through steam distillation, hydrodistillation, or cold pressing. During steam distillation, steam passes through plant material, extracting essential oil components, which are then condensed and separated. A by-product of this process is hydrolate (or floral water), which contains water-soluble components and retains a milder fragrance of the plant. Hydrolates are often used in aromatherapy and skin care due to their gentler properties compared to essential oils (3,4).

Although essential oils have been extensively characterized, hydrolates still require more attention in studies involving their chemical compositions. Regarding spagyric quintessences, analytical information is still limited, particularly in terms of their volatile chemical profiles and their comparability with conventional distillation products (5). Spagyric quintessences are preparations derived from spagyric and alchemical traditions, generally obtained through sequential processes such as distillation, fermentation, calcination, and recombination of fractions derived from plant material. Although these products are used in some traditional and complementary practices, analytical information on their chemical composition remains limited, especially regarding their volatile profiles and their comparability with conventional distillation products. The method involves separating the plant's essential oils, purifying its salts, and reassembling these components with spiritual and energetic elements, aiming to enhance the plant's therapeutic properties. Used in alternative medicine, spagyric quintessences are believed to treat not only the physical body but also the mental and spiritual aspects of the individual, promoting holistic healing (6).

From an analytical and regulatory perspective, understanding the chemical profiles of these different plant-derived products is essential to support rational use, guide practitioners, and avoid extrapolations not grounded in chemical evidence (1).

In this work, three plants used in integrative practices: geranium (*Pelargonium graveolens*), erva-baleeira (*Varronia curassavica*) and dentata lavander (*Lavandula dentata*) had their respective products (essential oil, hydrolate and quintessence) analyzed by chromatographic technique with the aim of comparing their chemical composition. This study is motivated by the need for clarity on the objectives of the applications of these products by therapists and users.

2. Material and Methods

2.1.1 Samples:

Commercial samples of essential oil and hydrolate from geranium (*Pelargonium graveolens*), erva-baleeira (*Varronia curassavica*), dentada lavander (*Lavandula dentata*) were kindly provided by Haje Insumos Orgânicos and the spagyric quintessence samples were kindly provided by Hermes Spagiria.

2.1.2 Hydrolate (HL) extraction:

The organic components of the hydrolates (HL) were extracted through partitioning using 250 mL of aqueous phase and 30 mL (3x) of petroleum ether. Salting out with NaCl was

applied. The ether was then evaporated using a rotary evaporator, and the resulting oil extracted was dried with Na_2SO_4 and weighed.

2.1.3 Sample preparation for analysis:

For chemical profile determination spagyric quintessence oils were filtered to remove carbonate salts. Essential sample oils, the extract obtained from hydrolate and filtered spagyric quintessence were diluted inside the vial with ethyl acetate in a proportion of 1:100 and after dilution they were taken to gas chromatography. Analyses were made on a Shimadzu QP2010 Plus (Tokyo, Japan) GC-MS system using a DB5-MS fused silica capillary column (30 m, 0.25 mm I.D., 0.25 μm film thickness). For chemical profile determination the oven temperature was programmed to rise from 60 °C to 280 °C at 3 °C/min and then hold at this temperature for 20 min. The carrier gas was He (99.999%) with a flow rate of 1.03 mL/min and injector and interface temperatures were maintained at 260 °C and 200 °C, respectively. After sample preparation for analysis 0.5 μL aliquots were injected in split mode (split ratio 1:50). Identification of the volatiles in quintessences, essential oil samples and oil extracted from hydrosols was based on a comparison of their mass spectra against the NIST 14 library. The retention indexes were calculated and compared to the ones listed in "Identification of essential oil components by Gas Chromatography/Mass Spectrometry" (7). The comparative analysis of essential oils (EO), hydrolates (HL) and spagyric quintessences (QE) was performed based on the relative chemical composition obtained by GC–MS. Each product was treated as a complex chemical mixture, and for each species a single compositional profile was considered, corresponding to the relative percentages of the identified volatile compounds. The analysis was descriptive and exploratory, focusing on the structural organization of the chemical profiles rather than on population-level inference. Identified compounds were grouped into three major chemical classes according to their dominant structural features: oxygenated terpenes (O), monoterpene hydrocarbons (M) and sesquiterpene hydrocarbons (S). For each product (EO, HL and QE), the relative abundances (%) of individual compounds were summed within each class, resulting in an O/M/S compositional distribution representing the global chemical signature of the product. Comparisons among products were carried out exclusively based on these relative class distributions. The results were visualized using stacked bar charts, generated in Python, in which each bar represents a product and each segment corresponds to the relative contribution of the O, M and S classes. This approach allows direct comparison among EO, HL and QE within each species and enables the identification of compositional similarity patterns (clustering) without the application of formal multivariate statistical algorithms.

3. Results

3.1 Chemical composition comparison

The chemical profiles obtained in this study showed that the hydrolate samples were predominantly composed of oxygenated compounds, whereas essential oils and spagyric quintessences exhibited broader volatile profiles.

Table 1: Chemical composition of *Lavandula dentata* essential oil (OE), hydrolate (HL) and spagyric quintessence (QE).

Substance	Kovats Index	OE(%)	HL(%)	QE(%)
α-pinene	935	3.63	0	3.2
camphene	953	0.88	0	0.84
verbenene	956	0	0	0.19
sabinene	973	0.96	0	0.43
β-pinene	979	5.49	0	4.66
myrcene	987	1.15	0	0.46
p-cymene	1024	0	0	0.55
limonene	1029	4.92	0	3.39
1,8-cineole	1033	34.31	4.68	38.97
fenchone	1087	14.45	11.34	14.35
cis-linalool oxide (furanoid)	1070	0	2.66	0
linalool	1096	2.51	2.74	2.3
endo-fenchol	1117	6.44	11.08	6.74
trans-pinocarveol	1140	0.7	3.02	0.89
camphor	1145	15.65	27,80	16.35
borneol	1170	1.71	9	1.14
cis-linalool oxide (pyranoid)	1171	0	1.93	0
terpinen-4-ol	1178	0.44	1.85	0.44
α-terpineol	1191	1.16	7.04	-
α-terpineol + myrtenol	1191	-	-	1.88
myrternal + myrtenol	1191	0.79	-	-
verbenone	1203	0	3.06	0
carvone	1240	0	0	0.19
thymol	1285	0	2.09	0
trans-α-bergamotene	1426	0.49	0	0.29
β-selinene	1481	0.9	0	0.42
β-bisabolene	1499	0.72	0	0.32
α-humulene	1450	2.16	0	0
caryophyllene oxide	1573	0	0	0.29

Analysis of the composition of the three *Lavandula dentata* samples (essential oil, hydrolate and quintessence) reveals a significant difference between the hydrolates and the other

two samples. In contrast, the essential oil and spagyric quintessence exhibit relatively similar compositions. For instance, the primary components of the essential oil and spagyric quintessence are 1,8-cineole (figure 1A) (34.31% and 38.97%, respectively), camphor (figure 1B) (15.65% and 16.35%, respectively), and fenchone (figure 1C) (14.45% and 14.35%, respectively). Conversely, the major components of the hydrolate are camphor (27.80%), fenchone (11.34%), and endo-fenchol (figure 1D) (11.08%). Regarding the products obtained from *L. dentata*, all major components are oxygenated monoterpenes. However, 1,8-cineole contains an ether functional group (known as oxide in aromatherapy literature), whereas camphor and fenchone are cyclic ketones, and endo-fenchol is a monoterpene with an alcohol function. It can be inferred that the more pronounced polarity of the alcohol functional group in endo-fenchol is the determining factor for the higher proportion of this molecule in the hydrolate (a polar aqueous solution). In contrast, the ether functional group in 1,8-cineole exhibits lower polarity than the ketone group, resulting in a lower affinity of 1,8-cineole for the hydrolate and a higher relative proportion of fenchone and camphor in this medium."

Table 2: Chemical composition of *Varronia curassavica* essential oil (OE), hydrolate (HL) and spagyric quintessence (QE).

Substance	Kovats Index	OE(%)	HL(%)	QE(%)
(Z)-3-hexenol	859	-	8.2	-
α-thujene	925	-	-	1.26
α-pinene	934	22.5	-	44.98
sabinene	972	1.78	-	0.75
β-pinene	978	4.33	-	1.86
myrcene	986	0.73	-	0.46
p-cymene	1023	-	-	0.56
limonene	1028	1.09	-	0.77
β-phellandrene	1029	-	-	0.38
1,8-cineole	1035	3.21	9.09	2.09
phenyl ethyl alcohol	1113	-	4.71	-
trans-pinocarveol	1142	-	15.02	-
trans-verbenol	1148	-	8.92	-
pinocarvone	1164	-	3.56	-
p-mentha-1,5-dien-8-ol	1169	-	4.18	-
terpene-4-ol	1179	-	10.42	-
α-terpineol	1191	-	2.1	-
myrtenol + myrtenal	1196	-	5.86	-
verbenone	1208	-	3.56	-
trans-carveol	1219	-	3.99	-
bornyl acetate	1279	1.01	-	1.2
δ-elemene	1329	25.97	-	1.68
citronellyl acetate	1344	0.25	-	0.53
β-elemene	1382	5.65	-	3.33

cis-α-bergamotene	1404	-	-	1.16
β-caryophyllene	1410	13.8	-	16.81
6,9-guaiadiene	1445	0.63	-	-
β-gurjunene	1421	-	-	0.55
α-humulene	1447	4.14	-	3.16
allo-aromadendrene	1451	1.08	-	6.06
γ-muurolene	1478	0.52	-	-
germacrene D	1482	2.33	-	-
ar-curcumene	1473	-	-	0.42
δ-selinene	1491	0.56	-	-
β-bisabolene	1498	-	-	2.13
germacrene B	1558	0.61	-	-
caryophyllene oxide	1571	0.3	-	6.54

The analysis of the results obtained for *Varronia curassavica* (erva-baleeira) samples reveals distinct profiles. In the essential oil, the three most prominent components are ***δ***-elemene (figure 1E) (25.97%), α-pinene (figure 1F) (22.50%), and β-caryophyllene (figure 1G) (13.80%). The spagyric quintessence is characterized by α-pinene (44.98%) and β-caryophyllene (16.81%) as major constituents. Finally, the hydrolate presents trans-pinocarveol (figure 1H) as major component (15.02%), followed by terpinen-4-ol (figure 1I) (10.42%), 1,8-cineole (9.09%), and trans-verbenol (figure 1J) (8.92%). Through comparative analysis, it can be inferred that the spagyric quintessence concentrates the most volatile major component of the essential oil (α-pinene). This result is expected due to the redistillation process used to obtain quintessence, which tends to select the more volatile fraction of the oil. Regarding the hydrolate, the chemical profile is markedly distinct from that of the essential oil. The hydrolate features four oxygenated monoterpenoids as major components. This finding is explained by the higher relative affinity of these components for water compared to the hydrocarbons that predominate in the respective essential oil.

Table 3: Chemical composition of *Pelargonium graveolens* essential oil (OE), hydrolate (HL) and spagyric quintessence (QE).

Substance	Kovats Index	OE **(%)**	HL**(%)**	QE**(%)**
(E)-2-hexenal	854	-	0.28	-
(Z)-3-hexenol	857	-	3.37	-
n-hexanol	866	-	0.59	-
6-methyl-5-hepten-2-one	986	-	0.14	-
(Z)-β-ocimene	1041	0.49	-	-
cis-linalool oxide (furanoid)	1073	-	1.68	-
trans-linalool oxide (furanoid)	1088	-	1.09	-
2-nonanone	1083	0.96	-	-
linalool	1091	23.58	26.5	5.64
cis-rose oxide	1105	-	-	1.37
trans-rose oxide	1123	-	-	0.5

menthone	1147	0.81	0.49	3.87
iso-menthone	1157	11.5	9.17	4.35
iso-menthol	1176	0.55	-	-
α-terpineol	1183	2.17	5.39	0.44
citronellol	1221	12.45	9.98	46.34
geraniol	1249	32.17	39.92	19.6
6,9-guaiadiene	1435	6.1	-	-
geranial	1263	-	-	0.41
citronellyl formate	1269	-	-	2.96
geranyl formate	1292	-	-	0.86
eugenol	1355	-	0.94	-
citronellyl acetate	1345	-	-	0.4
β-bourbonene	1377	-	-	1.48
trans-caryophyllene	1410	-	-	0.58
geranyl propanoate	1463	1.34	-	0.63
germacrene D	1472	0.64	-	-
γ-cadinene	1508	-	-	0.61
citronellyl butanoate	1518	-	-	0.66
geranyl butanoate	1551	0.56	-	-
2-phenyl ethyl tiglate	1574	-	-	0.56
10-epi-γ-eudesmol	1608	4.28	-	4.69
geranyl tiglate	1690	2.4	-	0.9
Substance	Kovats Index	OE **(%)**	HL**(%)**	QE**(%)**
(E)-2-hexenal	854	-	0.28	-
(Z)-3-hexenol	857	-	3.37	-
n-hexanol	866	-	0.59	-
6-methyl-5-hepten-2-one	986	-	0.14	-
(Z)-β-ocimene	1041	0.49	-	-
cis-linalool oxide (furanoid)	1073	-	1.68	-
trans-linalool oxide (furanoid)	1088	-	1.09	-
2-nonanone	1083	0.96	-	-
linalool	1091	23.58	26.5	5.64
cis-rose oxide	1105	-	-	1.37
trans-rose oxide	1123	-	-	0.5
menthone	1147	0.81	0.49	3.87
iso-menthone	1157	11.5	9.17	4.35
iso-menthol	1176	0.55	-	-

α-terpineol	1183	2.17	5.39	0.44
citronellol	1221	12.45	9.98	46.34
geraniol	1249	32.17	39.92	19.6
6,9-guaiadiene	1435	6.1	-	-
geranial	1263	-	-	0.41
citronellyl formate	1269	-	-	2.96
geranyl formate	1292	-	-	0.86
eugenol	1355	-	0.94	-
citronellyl acetate	1345	-	-	0.4
β-bourbonene	1377	-	-	1.48
trans-caryophyllene	1410	-	-	0.58
geranyl propanoate	1463	1.34	-	0.63
germacrene D	1472	0.64	-	-
γ-cadinene	1508	-	-	0.61
citronellyl butanoate	1518	-	-	0.66
geranyl butanoate	1551	0.56	-	-
2-phenyl ethyl tiglate	1574	-	-	0.56
10-epi-γ-eudesmol	1608	4.28	-	4.69
geranyl tiglate	1690	2.4	-	0.9

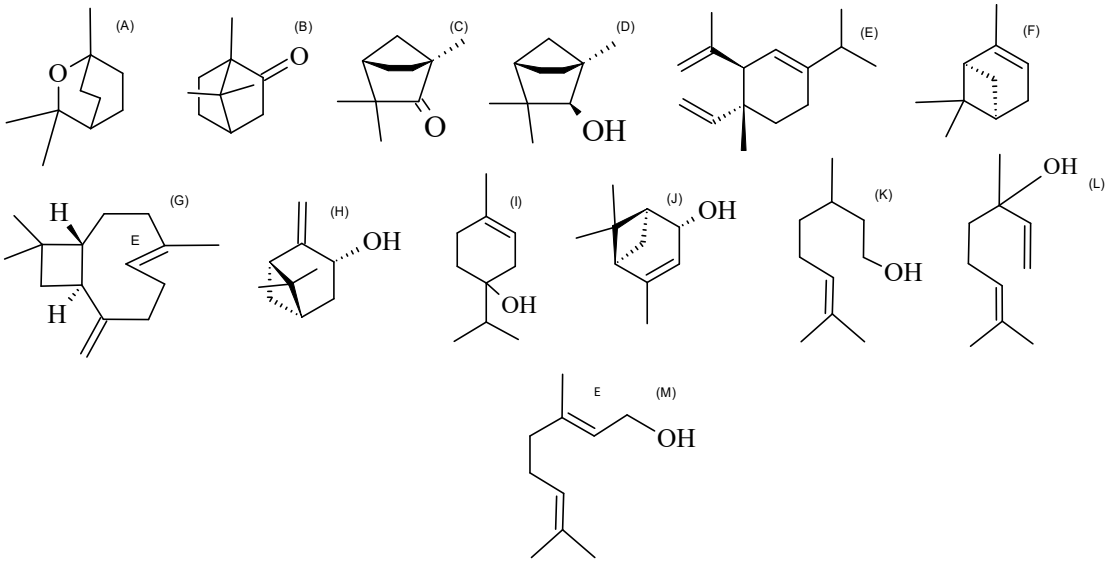

Fig 1: 1,8-cineol (A), camphor (B), fenchone (C), endo-fenchol (D), *δ*-elemene (E), α-pinene (F), β-caryophyllene (G), trans-pinocarveol (H), terpinen-4-ol (I), trans-verbenol (J), geraniol (K), linalool (L) and citronellol (M).

The analysis of the products obtained from *Pelargonium graveolens* revealed partially similar chemical profiles among the samples, with geraniol, linalool, and citronellol being among the major constituents. In the essential oil, the main compounds were geraniol

(32.17%), linalool (23.58%), and citronellol (12.45%). In the hydrolate, geraniol (39.92%) and linalool (26.50%) remained predominant, followed by citronellol (9.98%). In contrast, the spagyric quintessence showed a different distribution, with citronellol as the major constituent (46.34%), followed by geraniol (19.60%) and linalool (5.64%). These results indicate that, although the three products share important oxygenated monoterpenes, their relative proportions differ substantially according to the type of preparation.

3.2 Comparative compositional analysis

The comparative compositional analysis of essential oils (EO), hydrolates (HL) and spagyric quintessences (QE), based on the relative distribution of chemical classes, revealed consistent and interpretable patterns of similarity among these products (Figure 1). Although no formal multivariate clustering algorithms were applied, the stacked bar representations of oxygenated terpenes (O), monoterpene hydrocarbons (M) and sesquiterpene hydrocarbons (S) clearly evidenced compositional groupings that can be interpreted as clustering patterns, reflecting the dominant chemical structure associated with each product type.

Across all species analyzed, hydrolates formed a chemically distinct group characterized by a strong predominance of oxygenated terpenes (Figure 2A–C). This pattern reflects the preferential solubility of oxygenated compounds in the aqueous phase during hydrodistillation and has been consistently reported for hydrolates (8). In contrast, essential oils exhibited more complex and heterogeneous chemical profiles, with variable contributions of monoterpenes, oxygenated monoterpenes and sesquiterpenes depending on the botanical species (Figure 2).

Quintessences consistently displayed an intermediate compositional profile, generally clustering closer to essential oils than to hydrolates, while remaining chemically distinct from both (Figure 2A–C). This intermediate positioning suggests partial preservation or recombination of volatile constituents during spagyric processing steps, resulting in products that retain elements of the lipophilic fraction characteristic of essential oils while still being influenced by aqueous processing.

The degree of compositional similarity among EO, HL and QE were strongly species-dependent. In *Pelargonium graveolens*, all three products were dominated by oxygenated terpenes, resulting in a high level of structural coherence among EO, HL and QE (Figure 2A). This convergence indicates that, for this species, differences among products are primarily quantitative rather than qualitative, suggesting a higher degree of chemical comparability at the functional class level.

In *Lavandula dentata*, a more complex pattern was observed. Hydrolates were almost exclusively composed of oxygenated terpenes, whereas essential oils exhibited a more heterogeneous profile, including a relevant fraction of monoterpene hydrocarbons (Figure 2B). Quintessences showed an intermediate distribution, maintaining a high proportion of oxygenated terpenes while recovering part of the monoterpene fraction present in the

essential oil. This compositional behavior suggests that QE preserves a broader spectrum of volatile constituents than HL, resulting in greater chemical proximity to EO.

The most pronounced compositional redistribution among products was observed for *Varronia curassavica*. In this species, essential oils were dominated by sesquiterpenes, while hydrolates were almost exclusively composed of oxygenated monoterpenes, leading to a clear chemical separation between these products (Figure 2C). Quintessences again exhibited an intermediate profile, retaining both monoterpene and sesquiterpene fractions, which positions QE as a transitional product with greater chemical affinity to EO than to HL.

Taken together, these results demonstrate that chemical comparability among EO, HL and QE are not universal but highly dependent on the botanical species and on the physicochemical processes involved in product preparation. The compositional clustering observed in this study indicates that the processing method exerts a major influence on the global chemical structure of plant-derived products, often exceeding the influence of botanical origin when products are compared across product types.

From an applied and regulatory perspective, these findings highlight the limitations of using essential oils, hydrolates and spagyric quintessences interchangeably without prior chemical characterization. The analysis based on chemical classes proved to be an effective strategy for capturing global structural similarities and differences among complex mixtures, reinforcing the need for compositional evidence to support rational use and to avoid extrapolations not grounded in chemical data.

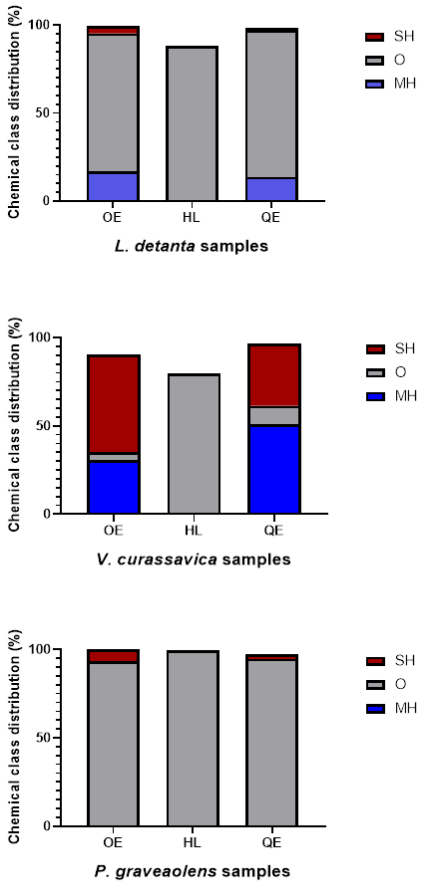

Fig 2. Chemical class distribution (oxygenated terpenes, monoterpene hydrocarbons and sesquiterpene hydrocarbons) in essential oils (EO), hydrolates (HL) and spagyric quintessences (QE) from *(A) Pelargonium graveolens*, *(B) Varronia curassavica* and *(C) Lavandula dentata*. Bars represent the relative contribution (%) of each chemical class, based on GC–MS compositional data.

4. Conclusion

Essential oils, hydrolates, and spagyric quintessences obtained from the same plant species showed distinct volatile chemical profiles. In general, hydrolates were enriched in oxygenated compounds, whereas essential oils and quintessences showed broader and more variable compositions. Quintessences often exhibited an intermediate profile, closer to essential oils than to hydrolates, although this pattern was species dependent. These findings indicate that these products should not be considered interchangeable without prior chemical characterization. Even when derived from the same botanical source, differences in processing can lead to relevant compositional changes, which should be considered in analytical interpretation and in discussions of their rational use.

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