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Composition of Essential Oils from Fruits of *Peucedanum longifolium* and *Rhizomatophora aegopodioides* (Apiaceae) with Regard to Other Related Taxa—A Chemometric Approach

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Abstract: The aim of this work was to investigate the composition of essential oils isolated from fruits of *Peucedanum longifolium*, and *Rhizomatophora aegopodioides* (a species which was previously placed in the genus *Peucedanum*), as well as to compare the obtained results to those available for other previously investigated related species (including taxa which are also, according to some authors, excluded from the genus *Peucedanum*). Essential oils were obtained via hydrodistillation in a Clevenger-type apparatus and their composition was analyzed using GC-FID and GC-MS. To compare these data to those of previously investigated taxa, a chemometric approach was applied; the data were analyzed using multivariate statistical methods: non-metric multidimensional scaling (nMDS) and hierarchical cluster analysis. The most abundant in *P. longifolium* essential oil were monoterpenes (79.7%), mostly α-phellandrene (26.2%), β-phellandrene + limonene (21.0%) and myrcene (9.5%), followed by sesquiterpenes (18.3%), mostly germacrene B (9.5%). On the other hand, dominant in *R. aegopodioides* essential oil were non-terpenic aliphatic hydrocarbons (46.1%), mainly *n*-undecane (16.5%) and *n*-nonane (11.3%). In addition, this essential oil also contained a notable quantity of sesquiterpenes (25.1%), with (*E*)-sesquilavandulol being the most abundant (10.0%). The results of multivariate statistics revealed a clear separation of the essential oil composition of *R. aegopodioides* and *P. longifolium*, as well as of *P. longifolium* and *P. officinale*. The clustering of the samples of most of the taxa that do not belong to the *Peucedanum* in the narrow sense (*sensu stricto*) was also observed, which is in accordance with their recent inclusion in separate genera.

Keywords: *Peucedanum longifolium*; *Rhizomatophora aegopodioides*; fruits; essential oils; GC-FID and GC-MS; nMDS; cluster analysis

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1. Introduction

The genus *Peucedanum* L. (Apiaceae, Selineae), in the broadest sense (*sensu amplo*), is taxonomically a very polymorphic and polyphyletic group with 2–3-pinnate leaves and dorsally compressed fruits, and historically 859 specific and intraspecific plant names are attributed to it [1], of which about 100–120 (200) species have been recognized [2,3]. Based on phylogenetic [4], and other studies [5], North American and African genera, as well as *Dichoropetalum* Fenzl and some Eurasian genera, have been excluded from it nowadays; so, there is a consensus that in a broad sense (*sensu lato*), this genus includes 74 species distributed in Eurasia and North Africa [6,7]. Phylogenetically, they form a common clade with the type species of the genus, *P. officinale* L. [4,8]. However, some authors claim that this group actually consists of eight independent genera that differ considerably in the morphology of the vegetative parts, chemistry, etc. [1,4,5,8–11]. Some of them are mono- or oligotypic and the genus *Peucedanum* in a narrow sense (*sensu stricto*) consists of only

12 Eurasian species, and 38 species need to be distributed into other genera [1]. More recently, it has been proven on the basis of molecular analyses [11] that the separation of the monotypic genus *Rhizomatophora* Pimenov from *Peucedanum sensu lato* is justified [7,9].

Many *Peucedanum* taxa, both in a broad sense (*sensu lato*) and in a narrow sense (*sensu stricto*), were the subject of previous phytochemical studies. The majority of these studies concerned essential oils and coumarins [12]. Essential oils were rich in monoterpenes, such as those of *P. officinale* rhizomes, stems, leaves, flowers and fruits [13,14], or in sesquiterpenes, for example, those of *P. tauricum* M. Bieb. flowers and fruits [15]. Also, in some instances, the essential oils of *Peucedanum* taxa contained similar amounts of both of these types of terpenes, such as the one of *P. verticillare* (L.) W.D.J. Koch ex DC. fruits [16]. Regarding coumarins, mainly simple coumarins, furanocoumarins and their dihydro derivatives, as well as dihydropyranocoumarins were identified in different extracts originating from these species. Among other secondary metabolites, flavonoids, phenolic acids, chromones and phenylethanoids were revealed in the polar extracts of these taxa [12].

In this paper, the composition of the essential oils isolated from the fruits of *Peucedanum longifolium* Waldst. & Kit., as well as *Rhizomatophora aegopodioides* (Boiss.) Pimenov [=*P. aegopodioides* (Boiss.) Vandas], was analyzed. Like other species of *Peucedanum sensu stricto*, *P. longifolium* has xeromorphic leaves and linear leaf lobes with entire margins, and inhabits rocky places in Southeast Europe and Southwest Asia. In contrast, *R. aegopodioides* has mesomorphic leaves with ovate to oblong and toothed leaf lobes, and inhabits moist riparian habitats in Southern Italy, Southeast Europe and Southwest Asia [1,7,17].

Previously, essential oils of various aerial parts and organs of *P. longifolium*, but not of fruits, from Serbia, Montenegro and Turkey were investigated. Also, the root essential oil of the plant collected in Serbia was analyzed [18–23]. Furthermore, for the aerial parts' essential oils (exact plant parts were not defined) from Turkey and Serbia, antioxidant and antibacterial activities, respectively, were demonstrated [18,19]. Also, furanocoumarins peucedanin, oxypeucedanin, oxypeucedanin hydrate and isoimperatorin, and simple coumarin osthole were isolated from the dry ethanol extracts of the roots and fruits of this plant [24].

Rhizomatophora aegopodioides' essential oil composition was not the subject of former studies. For the dry methanol, ethyl acetate, water and/or acetone extracts of the aerial parts of this plant (investigated under the name *Peucedanum aegopodioides*), antioxidant (in DPPH and ABTS tests), antibacterial and antifungal activities were demonstrated [25].

The aim of this work was to investigate the composition of the essential oils isolated from the fruits of *P. longifolium* and *R. aegopodioides*, as well as to compare these results using multivariate statistics to those available for other previously investigated related species, including taxa which are also, according to some authors, excluded from the genus *Peucedanum*.

2. Materials and Methods

2.1. Plant Material

Umbels with ripe fruits of 20 individual plants were collected: in the case of *P. longifolium* from a population on Vis hill in Sićevo Gorge (43.324110° N, 22.087002° E, SE Serbia) on 22 October 2022; and in the case of *R. aegopodioides* from a population in the vicinity of Pirot, near village Basara (43.157361° N, 22.680775° E, SE Serbia) on 6 September 2022. The plants were identified by Dr. Marjan Niketić, curator/botanist of the Natural History Museum, Belgrade (Serbia). The voucher specimens are deposited in the Herbarium of the Natural History Museum, Belgrade (BEO), under the numbers 4398/01 and 4566/01, respectively. For isolation of essential oils, ripe fruits removed from umbels after drying were used.

2.2. Isolation of Essential Oils

Dried and powdered ripe fruits were hydrodistilled for 2.5 h using a Clevenger-type apparatus, according to a procedure given in European Pharmacopoeia 11.0 [26]; collecting solvent: *n*-hexane. Essential oils were dried over anhydrous sodium sulfate, *n*-hexane was evaporated, and the oils were stored at 4 °C until analysis. In the case of both species, essential oils were isolated from 90 g of fruits (three hydrodistillations of 30 g of fruits). The content of essential oils was expressed as the mean ± standard deviation: 0.91 ± 0.008%, *w/w* (*P. longifolium*); and 0.02 ± 0.004%, *w/w* (*R. aegopodioides*).

2.3. GC-FID and GC-MS Analysis

The composition of the essential oils was analyzed on an Agilent 6890N Gas Chromatograph (Agilent Technologies, Palo Alto, CA, USA), equipped with a split/splitless injector, a capillary column (Agilent HP-5MS 30 m × 0.25 mm, 0.25 µm film thickness) and a flame ionization detector (FID), and coupled to an Agilent 5975C MS detector (GC-FID-MS). Injector temperature: 200 °C. FID temperature: 300 °C. Carrier gas: helium. Carrier gas flow: 1.0 mL/min. The oven temperature program: 60 to 280 °C at 3 °C/min (linear); final temperature held for 10 min. Split ratio: 1:10. Essential oils were dissolved in *n*-hexane (1.5%, *v/v*). Injected volume: 1 µL. MSD operated in EI mode at 70 eV. MSD transfer line temperature: 250 °C. MSD ion source temperature: 230 °C. MSD analyzer (single quadrupole) temperature: 150 °C. Range *m/z*: 35–550. Scan speed: 2.83 scans/sec. The analysis was carried out using the MSD ChemStation E.01.00.237 software. Linear retention indices (RIs) of the essential oils' components were calculated using the retention times obtained for the homologue series of *n*-alkanes (C_8–C_{40}) (Fluka, Buchs, Switzerland), which were ran under the same GC conditions. The identification of the compounds was based on the comparison of their RIs and mass spectra to those from the NIST/NBS 05, Wiley libraries 8th edition, and the literature [27]. The relative percentages of the essential oils' components were calculated from the peak areas, which were recorded using FID.

2.4. Statistical Analysis

To compare the chemical composition of the essential oils isolated from the fruits of *P. longifolium* and *R. aegopodioides*, as well as of 12 previously investigated related taxa (23 essential oil samples), multivariate statistical methods, non-metric multidimensional scaling (nMDS) and unweighted pair group arithmetic averages clustering (UPGMA) were applied. nMDS was performed to graphically delineate dissimilarities and grouping among taxa, and UPGMA was used for the agglomerative hierarchical cluster analysis. The analyses were based on the Bray–Curtis pairwise distance matrix and included the essential oils' components that were present in the relative quantities ≥ 1%. In total, 25 samples and 83 variables were assembled. To reduce the large differences between the data (relative percentages), they were coded in the following way [28]: value 1 for 0%, value 2 for quantities ≥ 1% and <2%, value 3 for quantities ≥ 2% and <5%, value 4 for quantities ≥ 5% and <10%, value 5 for quantities ≥ 10% and <20%, value 6 for quantities ≥ 20% and <40%, value 7 for quantities ≥ 40% and <60%, value 8 for quantities ≥ 60% and <80%, and value 9 for quantities ≥ 80%. The analysis was performed using software Statistica 6.0 (Statsoft Inc., Tulsa, OK, USA).

3. Results and Discussion

3.1. Chemical Composition of Peucedanum longifolium and Rhizomatophora aegopodioides Fruit Essential Oils

GC-FID and GC-MS analysis of the essential oils obtained from the fruits of *P. longifolium* and *R. aegopodioides* (Table 1) revealed the presence of 46 and 48 components, comprising 98.0 and 90.0% of the total essential oils, respectively.

Table 1. Chemical composition of essential oils of *Peucedanum longifolium* (PL) and *Rhizomatophora aegopodioides* (RA) fruits.

RI_{exp} [1]	RI_{lit} [2]	Compound [3]	PL (% [4])	RA (% [4])
900	900	*n*-Nonane	–	11.3
911	–	Nonene isomer	–	0.3
926	924	α-Thujene	0.5	–
934	932	α-Pinene	1.7	–
949	946	Camphene	0.3	–
974	969	Sabinene	4.1	–
978	974	β-Pinene	2.3	–
990	984	2-Pentyl furan	–	0.3
991	988	Myrcene	9.5	–
1008	1002	α-Phellandrene	26.2	–
1012	1008	δ-3-Carene	0.1	–
1017	1014	α-Terpinene	0.1	–
1026	1020	*p*-Cymene	7.9	–
1031	1024/1025	Limonene + β-Phellandrene	21.0	–
1036	1032	(*Z*)-β-Ocimene	0.1	–
1046	1044	(*E*)-β-Ocimene	0.6	–
1058	1054	γ-Terpinene	0.2	–
1067	1065	*cis*-Sabinene hydrate (IPP vs. OH)	0.1	–
1073	1067	*cis*-Linalool oxide (furanoid)	2.1	tr
1089	1084	*trans*-Linalool oxide (furanoid)	1.3	–
1089	–	Undecene isomer	–	1.0
1092	–	Undecene isomer	–	4.5
1093	1090	6,7-Epoxymyrcene	0.1	–
1100	1095	Linalool	0.1	–
1100	1100	*n*-Undecane	–	16.5
1104	–	Undecene isomer	–	0.9
1113	–	Undecene isomer	–	3.3
1122	1119	*trans*-*p*-Mentha-2,8-dien-1-ol	0.1	-
1158	1144	(2*Z*)-Nonen-1-al	–	0.3
1178	1174	Terpinen-4-ol	0.2	tr
1187	1183	Cryptone	0.3	–
1203	–	Phellandrene epoxide isomer	0.8	–
1205	1201	*n*-Decanal	–	0.2
1238	–	Phellandrene epoxide isomer	0.1	–
1271	1266	*n*-Decanol	–	0.3
1284	–	Tridecene isomer	–	1.0
1291	–	Tridecene isomer	–	1.2
1298	1300	*n*-Tridecane	–	0.4
1302	1298	Carvacrole	0.2	–
1375	1374	α-Copaene	0.1	tr
1385	1387	β-Bourbonene	0.2	-
1390	1388	1-Tetradecene	–	0.4
1392	1389	β-Elemene	0.6	-
1407	1408	Dodecanal	tr	0.4
1414	1411	2-epi-β-Funebrene	–	1.2
1420	1417	(*E*)-Caryophyllene	0.8	–
1434	1434	γ-Elemene	0.5	–
1443	1440	β-Barbatene	–	1.5
1444	1442	6,9-Guaiadiene	0.1	–
1452	1453	Geranyl acetone	–	0.4
1454	1452	α-Humulene	0.8	–
1456	1454	(*E*)-β-Farnesene	tr	1.7
1477	1478	γ-Muurolene	tr	0.6
1482	1484	Germacrene D	1.2	1.2
1487	1489	β-Selinene	1.4	–
1496	1498/1500	α-Selinene + Bicyclogermacrene	0.6	–

Table 1. *Cont.*

RI_{exp} [1]	RI_{lit} [2]	Compound [3]	PL (% [4])	RA (% [4])
1498	1500	Pentadecane	–	0.5
1508	1502	*trans*-β-Guaiene	1.8	–
1509	1500/1505	Cuparene + β-Bisabolene	–	3.9
1524	1522	δ-Cadinene	0.1	0.8
1531	1533	*trans*-Cadina-1,4-diene	–	0.5
1560	1559	Germacrene B	9.5	–
1569	1565	Dodecanoic acid	–	1.3
1578	1577	Spathulenol	tr	0.3
1584	1582	Caryophyllene oxide	0.2	–
1602	1582	Neryl isovalerate	–	0.6
1610	1608	Humulene epoxide II	0.2	–
1633	1631	(*E*)-Sesquilavandulol	–	10.0
1680	–	Heptadecene isomer	–	1.0
1684	1685	α-Bisabolol	–	1.3
1691	–	Heptadecene isomer	–	0.6
1721	1714	(2*E*,6*Z*)-Farnesol	–	0.6
1766	–	Tetradecanoic acid	–	1.7
1844	–	Hexahydrofarnesyl acetone	–	1.4
1864	–	Pentadecanoic acid	–	0.5
1975	1959	Hexadecanoic acid	–	9.6
2138	–	Octadecadienoic acid isomer	–	1.2
2144	–	Octadecadienoic acid isomer	–	1.2
2147	–	Octadecenoic acid isomer	–	1.0
2296	2300	*n*-Tricosane	–	0.5
2497	2500	*n*-Pentacosane	–	1.9
2696	2700	*n*-Heptacosane	–	0.9
		Monoterpene hydrocarbons	74.4	–
		Oxygenated monoterpenes	5.4	1.1
		Sesquiterpene hydrocarbons	17.9	11.4
		Oxygenated sesquiterpenes	0.4	13.6
		Other aliphatic hydrocarbons	–	46.1
		Other oxygenated aliphatic hydrocarbons	tr	1.4
		Fatty acids	–	16.4
		Total identified compounds	98.0	90.0
		Number of identified compounds	46	48

[1] RI_{exp}, retention indices on HP-5MS column relative to C_8-C_{40} *n*-alkanes. [2] RI_{lit}, retention indices obtained from the literature [27]. [3] Constituents listed in the order of elution on HP-5MS column. [4] Relative area percentage of the compounds obtained from FID area percent data; tr, trace (<0.1%); –, not detected.

The *P. longifolium* fruit essential oil was dominated by monoterpene hydrocarbons (74.4%). The most abundant was α-phellandrene (26.2%), and it was followed by β-phellandrene and limonene (21.0%), which eluted together under applied GC conditions. It should be noted that the co-elution of these two compounds was also observed in several other studies on the essential oils of the fruits of the *Peucedanum* taxa [29–31]. Other monoterpene hydrocarbons present in the investigated *P. longifolium* fruit essential oil in notable amounts were myrcene (9.5%), *p*-cymene (7.9%) and sabinene (4.1%). Among sesquiterpene hydrocarbons, which also constituted a prominent portion of this essential oil (17.9%), germacrene B was the only one present in a noteworthy amount (9.5%). All other compounds were detected in quantities below 2.5%.

Essential oils of some other plant parts and organs of *P. longifolium* were investigated previously. Five of six of these studies investigated essential oils isolated from the aerial parts of this plant. The essential oil of leaves and young stems collected in eastern Serbia (Mt. Tupižnica) was dominated by sesquiterpene β-elemene (24.7%), followed by monoterpene (*E*)-β-ocimene (11.7%) [20]. A similar composition was observed for the essential oils isolated from the leaves, collected in two phenophases (vegetative and flowering), also in eastern Serbia (Mt. Stara Planina), i.e., β-elemene (44.1 and 22.5%) and (*E*)-β-ocimene (8.5 and 26.7%) were also the most abundant. On the other hand, the flower essential oil of the plant collected on the same locality was rich in monoterpenes myrcene (23.1%), α-phellandrene (22.5%) and β-phellandrene (16.4%) [21]. Similarly, these three compounds were among the dominant in the fruit essential oil analyzed in our study. However, in the fruit essential oil, α- and β-phellandrene were more abundant than myrcene. In the three remaining studies, the aerial parts were not precisely defined. The essential oil of those collected in eastern Serbia (Mt. Rtanj) was dominated by myrcene (15.9%) and α-phellandrene (11.3%) [19]. The amount of myrcene could indicate that these aerial parts included flowers, but studies on more samples of flowers and fruits are necessary to prove this hypothesis. The essential oil of the aerial parts from Montenegro was also dominated by monoterpenes; however, the most abundant was α-pinene (36.3%) [22], while in the essential oil of the aerial parts from Turkey, the dominant was a sesquiterpene 8-cedren-13-ol (33.7%) [18]. Besides the aerial parts essential oils, in one study, the essential oil of the roots (collected on Mt. Stara Planina in eastern Serbia) was investigated. α-Pinene (60.3%) and sabinene (20.9%) were dominant [23].

In contrast to the *P. longifolium* fruit essential oil, the most abundant in the *R. aegopodioides* fruit essential oil were non-terpenic aliphatic hydrocarbons (46.1%), mainly *n*-undecane (16.5%) and *n*-nonane (11.3%). This essential oil also contained significant amounts of both non-oxygenated and oxygenated sesquiterpenes (11.4 and 13.6%), with (*E*)-sesquilavandulol being the most prominent (10.0%). A notable quantity of hexadecanoic acid (9.6%) was also present in *R. aegopodioides'* fruit essential oil. Other compounds were detected in amounts below 5.0%.

3.2. Composition of Peucedanum longifolium and Rhizomatophora aegopodioides Fruit Essential Oils with Regard to Related Taxa

To compare the chemical composition of the essential oils obtained from the fruits of *P. longifolium* and *R. aegopodioides*, as well as of other related taxa, a chemometric approach was applied. The search for previous studies was performed using Google Scholar on 15.11.2023 using input text "*Peucedanum*" and "essential oil" and "fruit". Also, the search was repeated, but using "seed" instead of "fruit", because some authors incorrectly refer to fruits of the Apiaceae species as seeds. Moreover, a similar query was performed for the genera which are, according to some authors, excluded from *Peucedanum*, i.e., for *Rhizomatophora*, *Xanthoselinum*, *Pteroselinum*, *Cervaria*, *Dichoropetalum*, *Oreoselinum*, *Thysselinum*, *Leutea*, *Tommasinia*, *Agasyllis*, *Pinacantha*, *Macroselinum*, *Paraligusticum*, *Karatavia*, *Imperatoria*, *Dystaenia*, *Leiotulus*, *Steganotaenia*, *Scandia*, *Annesorhiza*, *Lomatium*, *Ducrosia*, etc. In these instances, the data on the fruit essential oil composition were found only in the last six genera. However, in this paper, we limited ourselves only to representatives of the Selineae tribe [10] that grow in Europe, with the exception of the Asian genus *Leutea* (Scandiceae tribe), which was taken as an outgroup. The results of 14 appropriate previous studies (Table 2) were included in multivariate statistical analysis. In total, together with the results of our investigation, 25 fruit essential oil samples obtained from 14 taxa, containing 83 compounds in a quantity above 1%, were included in the analysis. The accepted names of the analyzed taxa (including *P. longifolium* and *R. aegopodioides*), according to some authors, are given in Table 2. Of the 14 names, ten belong to *Peucedanum* in the broad sense (*sensu lato*), including five from *Peucedanum* in the narrow sense (*sensu stricto*). The dominant constituents of the fruit essential oils of these plants are also included in Table 2.

In the statistical analysis (Figures 1 and 2), a clear distinction of *R. aegopodioides'* fruit essential oil (aeg sample), dominated by non-terpenic aliphatic hydrocarbons, from that of other analyzed taxa, in which various terpenes were the main fruit essential oils' components, was demonstrated.

Table 2. Accepted names of the analyzed taxa according to Plants of the World Online (POWO) [7], and Catalogue of Life (COL) [1], as well as the most abundant constituents (≥5%) of their fruit essential oils.

Name Reported in Cited Article [Acronym]	Accepted Name in POWO	Accepted Name in COL	The Most Abundant Constituents in the Fruit Essential Oils (%)	Reference
Peucedanum alsaticum L. [als1] [1]	As in cited article	*Xanthoselinum alsaticum* (L.) Schur subsp. *alsaticum*	Sabinene (22.0), α-pinene (20.7), limonene + β-phellandrene (18.7), germacrene D (7.9), bornyl acetate (5.6), (*E*)-caryophyllene (5.5)	Skalicka-Woźniak et al. [29]
Peucedanum alsaticum L. [als2-4] [1]			α-Pinene (10.7–40.2), β-phellandrene (12.3–31.5), sabinene (15.7–33.9), γ-terpinene (2.4–5.8), camphene (1.6–5.7)	Chizzola [30]
Peucedanum austriacum (Jacq.) W.D.J. Koch [aus] [1]	As in cited article	*Pteroselinum austriacum* (Jacq.) Rchb.	β-Phellandrene (45.2), α-pinene (10.1), germacrene D (6.4), (*E*)-caryophyllene (6.1), germacrene B (5.6)	Jovanović et al. [32]
Peucedanum cervaria (L.) Lapeyr. [cer1]	As in cited article	*Cervaria rivini* Gaertn.	α-Pinene (31.3), sabinene (31.0), β-pinene (21.7)	Skalicka-Woźniak et al. [31]
Peucedanum cervaria (L.) Lapeyr. [cer2]			β-Pinene (33.1), α-pinene (22.3), sabinene (22.0), limonene + β-phellandrene (8.4)	Chizzola [30]
Peucedanum chryseum (Boiss. & Heldr.) Chamberlain [chr]	*Dichoropetalum chryseum* (Boiss. & Heldr.) Pimenov & Kljuykov	*Dichoropetalum chryseum* (Boiss. & Heldr.) Pimenov & Kljuykov	α-Pinene (72.8), β-pinene (20.4)	Ağalar et al. [33]
Peucedanum dhana Buch.-Ham. ex C.B. Clarke [dha] [1,2]	As in cited article	As in cited article	*trans*-Piperitol (51.2), β-pinene (11.7), *o*-cymene (11.1), γ-terpinene (9.2)	Khruengsai et al. [34]
Peucedanum officinale L. [off] [1,2]	As in cited article	As in cited article	Fenchone (32.0), (*E*)-β-ocimene (17.8), (*Z*)-β-ocimene (9.4), γ-terpinene (6.8), *p*-cymene (6.3), α-acorenol (5.0)	Jaimand et al. [14]
Peucedanum oreoselinum (L.) Moench [ore1] [1]	As in cited article	*Oreoselinum nigrum* Delarbre	Limonene (17.9), α-pinene (17.7), sabinene (16.5), β-pinene (14.4), (*Z*)-β-ocimene (12.9)	Silva et al. [35]

Table 2. *Cont.*

Name Reported in Cited Article [Acronym]	Accepted Name in POWO	Accepted Name in COL	The Most Abundant Constituents in the Fruit Essential Oils (%)	Reference
Peucedanum oreoselinum (L.) Moench [ore2-8] [1]			Four samples: limonene (44.1–56.6), γ-terpinene (12.2–17.5), β-pinene (8.5–14.5), α-pinene (5.1–8.3), α-phellandrene (3.5–4.1); two samples: limonene (76.0–82.4), sabinene (4.6–8.0), α-pinene (4.0–6.3)	Motskute & Nivinskene [36]
Peucedanum palustre (L.) Moench [pal] [1]	As in cited article	*Thysselinum palustre* (L.) Hoffm.	Limonene (87.5), γ-terpinene (9.1)	Schmaus et al. [37]
Peucedanum petiolare (DC.) Boiss. [pet]	*Leutea petiolaris* (DC.) Pimenov	*Leutea petiolaris* (DC.) Pimenov	α-Pinene (47.3), sabinene (45.9)	Mirza et al. [38]
Peucedanum ruthenicum M.Bieb. [rut] [1,2]	As in cited article	As in cited article	Caryophyllene oxide (13.6), 8,9-dehydroisolongifolene (11.3), 1,8-cineole (11.1), (*Z*)-carveol (6.9), camphor (5.9), carvone (5.6), caryophylla-4(12),8(13)-dien-5-β-ol (5.2)	Alavi et al. [39]
Peucedanum tauricum M.Bieb. [tau] [1,2]	As in cited article		Guaia-9,11-diene (28.6), guaia-1(10),11-diene (26.1)	Bartnik [15]
Peucedanum verticillare (L.) W.D.J.Koch ex DC. [ver] [1]	As in cited article	*Tommasinia altissima* (Mill.) Reduron	(*E*)-Caryophyllene (24.2), α-phellandrene (20.8), (*Z*)-β-farnesene (12.8), β-bisabolene (9.0), β-cubebene (7.5), caryophyllene oxide (6.7), α-*trans*-bergamotene (5.3), geranyl acetate (5.0)	Fraternale et al. [16]
Peucedanum longifolium Waldst. & Kit. [lon] [1,2]	*Peucedanum officinale* subsp. *longifolium* (Waldst. & Kit.) R.Frey	As in current work	α-Phellandrene (26.2), β-phellandrene + limonene (21.0), myrcene (9.5), germacrene B (9.5), *p*-cymene (7.9)	Current work
Rhizomatophora aegopodioides (Boiss.) Pimenov [aeg]	As in current work	As in current work	*n*-Undecane (16.5), *n*-nonane (11.3), (*E*)-sesquilavandulol (10.0), hexadecanoic acid (9.6)	Current work

[1] *Peucedanum* in the broad sense (*sensu lato*). [2] *Peucedanum* in the narrow sense (*sensu stricto*).

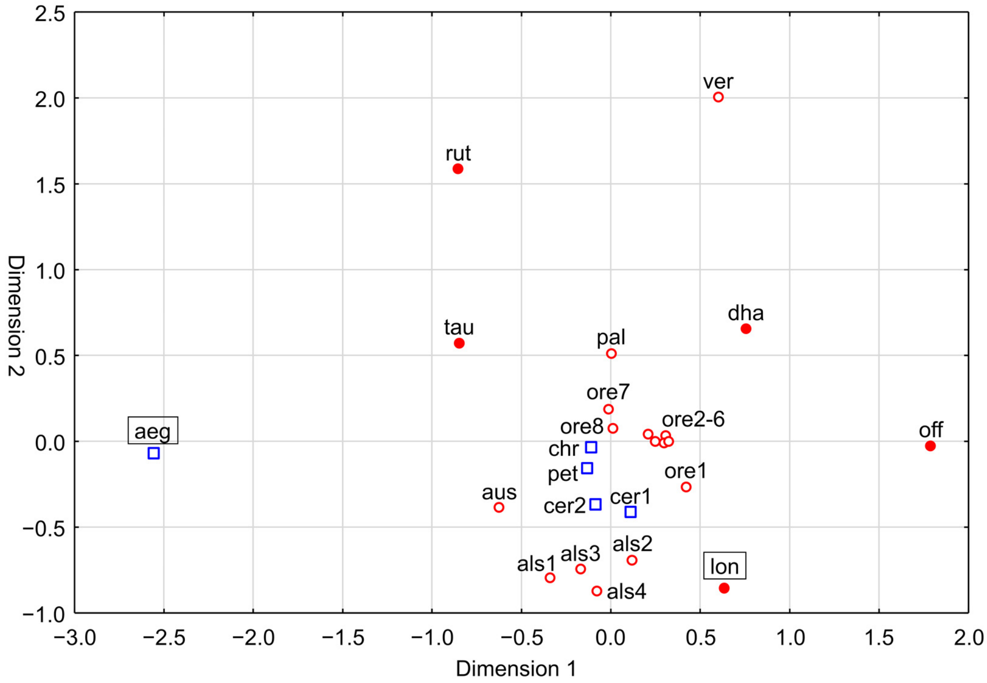

Figure 1. nMDS analysis of the composition of the fruit essential oils. *Peucedanum sensu lato* taxa are represented with circles with red outline and those that represent *Peucedanum sensu stricto* taxa are completely colored in red. Taxa that do not belong to *Peucedanum sensu lato* are represented with squares with blue outline. Acronyms are given in Table 2. Acronyms of samples investigated in the current work (lon and aeg) are outlined. Analysis was performed using coded values of relative % of the compounds: value 1—not detected, value 2—quantities ≥ 1% and <2%, value 3—quantities ≥ 2% and <5%, value 4—quantities ≥ 5% and <10%, value 5—quantities ≥ 10% and <20%, value 6—quantities ≥ 20% and <40%, value 7—quantities ≥ 40% and <60%, value 8—quantities ≥ 60% and <80%, value 9—quantities ≥80%.

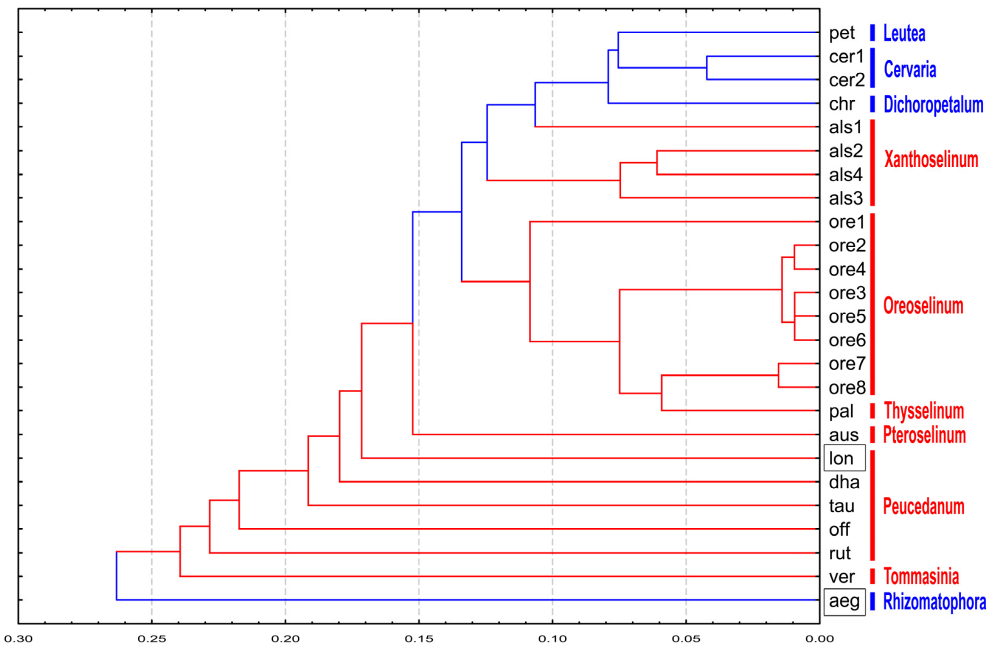

Figure 2. UPGMA cluster analysis of the composition of the fruit essential oils. *Peucedanum sensu lato* taxa are marked with red color and other taxa with blue color. Acronyms are given in Table 2. Acronyms of samples investigated in the current work (lon and aeg) are outlined. Coded values of relative % of the compounds used for analysis are given in Figure 1 caption.

Furthermore, the grouping of the essential oil samples of most of the other taxa (except the ver sample) that also do not belong to the *Peucedanum* in the narrow sense (*sensu stricto*) was observed. These essential oils were rich in monoterpene hydrocarbons. In most cases, α-pinene was amongst the dominant constituents (up to as much as 72.8%). Namely, α-pinene (10.7–40.2%), β-phellandrene (12.3–31.5%) and sabinene (15.7–33.9%) were the most abundant in *P. alsaticum* (now belonging to the genus *Xanthoselinum*) oil samples, α-pinene (31.3 and 22.3%), sabinene (31.0 and 22.0%) and β-pinene (21.7 and 33.1%) in *P. cervaria* (now belonging to the genus *Cervaria*) oil samples, α-pinene (72.8%) and β-pinene (20.4%) in *P. chryseum* (now belonging to the genus *Dichoropetalum*) oil sample, and α-pinene (47.3%) and sabinene (45.9%) in *P. petiolare* (now belonging to the genus *Leutea*) oil samples [29–31,33,38]. In addition, the *P. chryseum* and *P. petiolare* fruit essential oils generally had a small number of compounds (i.e., four) in a quantity above 1%, all of which were monoterpenes [33,38]. Further, the *P. oreoselinum* (now belonging to the genus *Oreoselinum*) and *P. palustre* (now belonging to the genus *Thysselinum*) fruit essential oil samples were also dominated by monoterpenes; however, the dominant one was limonene (17.9–87.5%) [35–37]. Regarding amounts of sesquiterpenes in all these essential oil samples, they were notably lower (below 9.0%) [29–31,33,35–38]. Somewhat different were the fruit essential oils of *P. austriacum* (now belonging to the genus *Pteroselinum*) and particularly *P. verticillare* (now belonging to the genus *Tommasinia*). These two, besides monoterpenes β-phellandrene (45.2%) and α-phellandrene (20.8%), respectively, also contained notable amounts of sesquiterpenes, such as germacrene D (6.4%) and (*E*)-caryophyllene (24.2%), respectively [16,32].

Within *Peucedanum sensu stricto*, the *P. longifolium* and *P. officinale* fruit essential oils (lon and off samples, respectively) were well separated, which does not support the opinion of some authors that *P. longifolium* is a subspecies of *P. officinale*. While the *P. longifolium* fruit essential oil sample was dominated by monoterpene hydrocarbons, in the *P. officinale* fruit essential oil sample, oxygenated monoterpene fenchone was the most abundant (32.0%) [14]. Our study represents a good basis for further research in this regard on more *P. longifolium* and *P. officinale* essential oil samples. Another oxygenated monoterpene *trans*-piperitol (51.2%) was the dominant in the fruit essential oil sample of *P. dhana* [34], which is also a member of *Peucedanum sensu stricto*. The remaining *Peucedanum sensu stricto* fruit essential oil samples investigated were dominated by sesquiterpenes: the *P. ruthenicum* essential oil was dominated by caryophyllene oxide (13.6%) and 8,9-dehydroisolongifolene (11.3%) [39], and the *P. tauricum* essential oil was dominated by guaia-9,11-diene (28.6%) and guaia-1(10),11-diene (26.1%) [15]. The *P. longifolium* fruit essential oil also contained a prominent amount of sesquiterpenes, mainly germacrene B.

It seems that small amounts of terpenic compounds in the fruit essential oil, as was the case in the *Rhizomatophora* sample, support the exclusion of such taxa from the *Peucedanum* genus. More studies are necessary to test the hypothesis that ratios of monoterpenes and sesquiterpenes, as well as of oxygenated and non-oxygenated terpenes, could also have the same role.

4. Conclusions

In this work, the composition of the essential oils obtained from the fruits of *Peucedanum longifolium*, as well as *Rhizomatophora aegopodioides* (which was previously a member of the genus *Peucedanum*), was investigated.

A multivariate statistical analysis of these results and appropriate literature data for the fruit essential oils of other related taxa was performed. An applied chemometric approach revealed the clustering of the samples of most of the taxa that do not belong to the *Peucedanum* in the narrow sense (*sensu stricto*), which is in agreement with their recent inclusion in separate genera. In this regard, significant differences were also revealed between the essential oils of *R. aegopodioides* and other taxa, including *P. longifolium*. The chemical composition of the essential oils analyzed also suggested the independent status of *P. longifolium* in relation to *P. officinale*.

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