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COMPARATIVE INVESTIGATION OF COLD PRESSED ESSENTIAL OILS FROM PEEL OF DIFFERENT MANDARIN VARIETIES

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ABSTRACT

The object of this study was to investigate the composition of different varieties of cold pressed mandarin peel oils by using Gas Chromatography-Mass Spectrometry. Results obtained from this study showed the major volatile compounds counting for >90% of total volatile flavour compounds. Identification and quantification of the volatiles indicated the most abundant compounds as monoterpene hydrocarbons (limonene, sabinene, β-pinene, γ-terpinene, myrcene, α-pinene and α-terpinolene), following by esters (methyl antranilate, neryl acetate and geranyl acetate), alcohols (linalool) and aldehyde compounds (decanal, α-sinensal, β-sinsnal and peril aldehyde). Principle component analysis (PCA) was employed to discriminate among the cold pressed mandarin oils based on their varieties and to evaluate their sensorial attributes. Results from PCA analysis showed classification of the samples of red mandarin oil from South Africa and unknown region in the same grope which was separated from yellow and sweet "Murcot" mandarin oil.

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KEY WORDS

Diabetic Cold pressed mandarin oil, esters, alcohols, GC-MS, alkanes, principle component analysis (PCA).

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[I] INTRODUCTION

Cold pressed citrus oils represent a large portion of the world market for flavour ingredients, food industry, and aromatherapy as well as perfume industry [1]. An expanding market for mandarin flavoured drinks uses the oils of lemon, orange, mandarin, grapefruit and bitter orange [2]. The flavour of citrus oils is usually defined as refreshing, green, citrus and it is extremely important for the flavouring of food, beverages, confectionary, cookies and dessert. From this point of view, the main role of mandarin oils is covering the "off flavor" in lemon and orange drinks.

Chemical composition of the cold-pressed citrus includes different volatiles, such as terpenes and oxygenated compounds, and nonvolatiles, such as waxes and pigments [3-10]. Terpene content should be minimal in order to protect the oils from oxidation. The most dominant monterpene limonene does not contribute to the overall flavor of mandarin oil and it high concentration (usually over 90 %) is responsible for oil instability as well as unpleasant "off" flavor. Furthermore, most of the volatile compounds can provide antifungal activity of oils [11-14]. Except gas chromatography, other analytical techniques were applied for examination of volatile compounds of citrus peel oils [15, 16].

The chemical composition of the citrus oils is usually affected to the geographical region and micro-ecological environment. In the work of Vercera et al., the chemical composition of two varieties of Nova and Satsuma peel mandarin oils from Urugvay was object of study [17]. Effect of geographical origin to the volatiles of different lemon peel oils was object of study in the work of Kostadinović et al. [18].

The flavor and the taste typical for "sweet mandarin", as in other citrus, is provided by oxygenated terpenes such as alcohols, esters and aldehydes. These volatile compounds can be "the key" for the overall flavor of mandarin oil even in the concentration less than 1%. Cold pressed mandarin oil usually is used as a blend with other citrus oils as orange and lemon or as a mask for unpleasant flavor in the food, aromatherapy and perfume industry [19, 20].

The first objective of the present study was investigation of the effect of variety on the composition of different cold pressed mandarin oils.

The second objective of the study was classification of the four samples of cold pressed mandarin oils regarding their volatile composition. Results from the percentage of the compounds

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were submitted to Principal Component Analysis (PCA) in order to find relationship between abundance of the volatiles and variety of the mandarin from which the peel oil was cold-pressed.

[II] MATERIALS AND METHODS

2.1. Samples of cold pressed mandarin oils

The four commercial samples of cold pressed mandarin oils were obtained from Aromaceuticals (Texas, United States).

2.2. Apparatus

The flavour compounds of three varieties cold pressed mandarin oils (red, yellow and sweet "Murcot") were analyzed using a Hewlett-Packard 6890 GC equipped with a Mass Spectrometer (MS) and an HP-5 cross-linked fused-silica capillary column (i.d. = 0.25 mm, length = 30 m, film thickness = 0.25 μm) supplied by Agilent inc. (PA, USA). In qualitative and quantitative analyses, 0.2 μl of cold pressed mandarin oil was injected in the split mode (1:100). Oven temperature was programmed at 40°C isothermally for 5 min, then ramped to 180°C at 4°C/min and then increased to 260°C at 20°C/min and held for 10 min at the final temperature. Helium was used as the carrier gas with a flow-rate of 5.3 (ml/min). Injector and detector temperatures were set at 270 and 300°C, respectively. The volatile flavour compounds were initially detected and confirmed using a Hewlett-Packard 6890N GC system (Wilmington, DE) and the NIST library version 2.0. The components of the essential oil were identified by comparison of their linear retention indices, determined in relation to a homologous series of n-alkanes (C8-C32), with those from pure standards or reported in literature. Comparison of fragmentation patterns in the mass spectra with those stored on databases and MS data of our collection was also performed.

2.3. Statistical analysis

On Principal component analysis (PCA) was performed to gain an overview of how the samples were correlated to each other with regard to equilibrium volatile headspace concentration. Correlation matrix was applied in multivariate analysis with Minitab software release 14 so that the data was autoscaled by variable to give the same weight to all components

[III] RESULT AND DISCUSSION

The volatile fraction composition of cold pressed essential oils from the peel of different specious of mandarin was studied using GC-MS. The obtained TIC chromatogram is presented in **Figure–1**. More than seventy components were identified and quantified using mass spectra and linear retention indices presented in **Supplementary Table-1**. The monoterpene limonene was the most abundant component even though not in a quantity expected for fresh mandarin oil. Relatively lower quantity of limonene suggested other extraction procedures apart from cold pressing for protecting the oils from oxidation [21]. α-pinene and α-tujene were the most abundant compounds after limonene responsible for the flavor of the mandarin oil. α-copaene, trans-α-bergamotene and β-farnesene were the most important sesquiterpenes responsible for the sweet taste of the "murcot" mandarin oil [22]. Octanal, nonanal, decanal from aliphatic aldehydes and geranial and α-sinensal from the class of monoterpene aldehydes were dominant in all samples of mandarin oils. Methyl antranylate was the main ester which contributes the most to the overall aroma of mandarin oil. Linalool was the major alcohol responsible for the sweet and floral smell of the oil. Significant quantity of flavones was detected around 250°C during chromatographic analysis. Polyphenolic compounds 4',5,6,7,8,-penthamethoxy flavone (tangeretin), 3,3',4',4,5,5'7,8-heptamethoxy flavone and 3',4',5,6,7,8-hexamethoxy flavone (nobiletin) in the role of natural antioxidants protected the oils from oxidation.

Regarding the total quantities of chemical classes of the volatile compounds sesquiterpenes, alcohols and aldehydes were the most dominant of volatiles in all samples of the oils **[Figure– 2]**. Red mandarin oil from South Africa had the highest quantities of esters and oxides which can be indication of oxidized oil. Acids and ketones were the least abundant compounds which contribute to the chemical composition of mandarin oils. Oils pressed from the peel of yellow mandarin and red mandarin from South Africa contained higher quantities of flavones which acts as natural antioxidants and protect the oils from oxidation. Nobiletine (3',4',5,6,7,8-hexamethoxy flavone) was the most abundant flavone in examined samples of mandarin oils.

However, the quantitative information summarized in **Supplementary Table-1** and **Figure– 1** was not enough to evaluate the similarities and differences between the cold pressed mandarin oils considered in this study.

A multivariate pattern recognition approach should be more effective in recognizing differences among the samples analyzed. The results showed the comparison between the major chemical classes of volatile chemical compounds of three varieties of cold pressed mandarin oils **[Supplementary Table-1]**. Apart from monoterpenes as the most abundant group of volatiles, three varieties of cold pressed mandarin oil had the highest quantities of sesquiterpenes, alcohols and aldehydes. Esters and oxides were present in lower quantities and the least abundant were acids, ketones and flavones. Sesquiterpenes are a major group of flavour compounds in citrus oils in term of quantity.

PCA score plots were used to determine whether for different cold pressed mandarin oils could be grouped into different classes **[Figure– 3]**. To focus on the differences among the cold pressed mandarin oils and target volatile compounds, cluster observation and cluster variable dendrograms were constructed using the nearest neighbour **[Figure– 3]**. The results indicated that first two principal components explained 97.1% and 2.7% of the total variability, respectively. Despite first two principal components, which showed 99.8% of total variation, the remaining principal components didn't account for any variability and were probably unimportant.

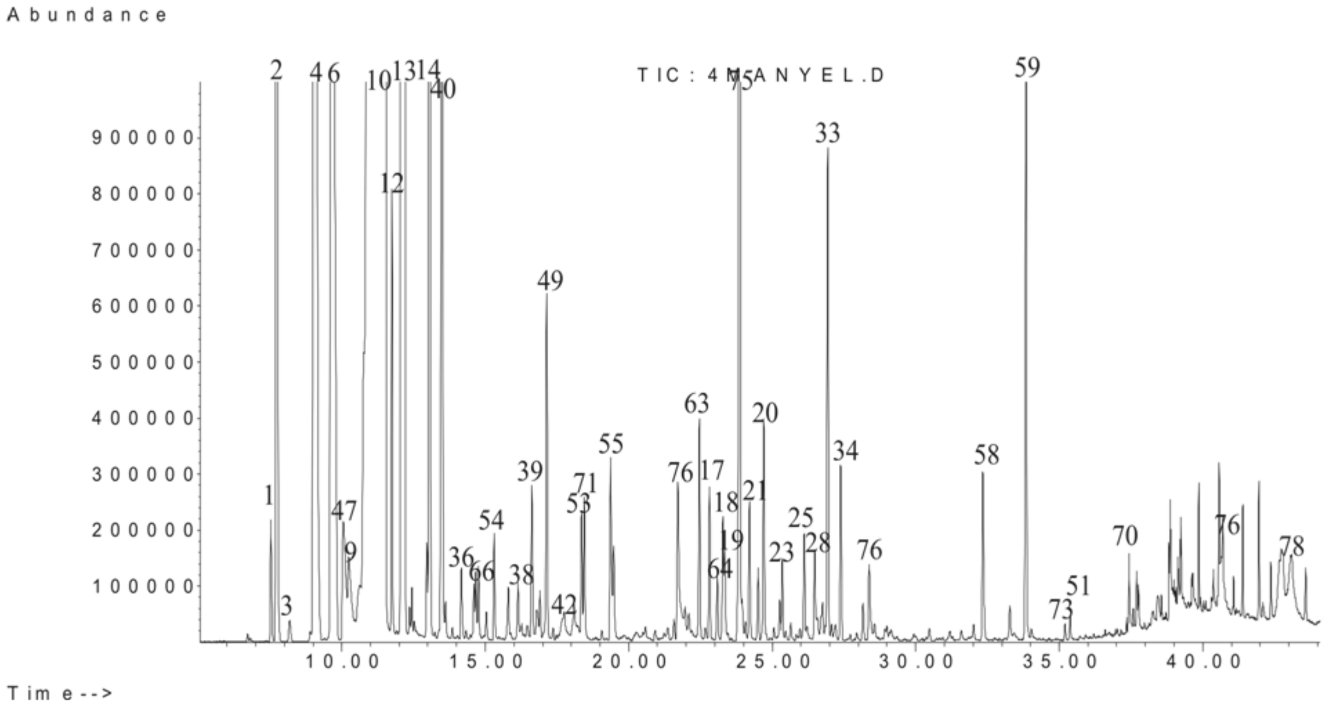

Fig.1. TIC chromatogram of cold pressed "yellow" mandarin oil

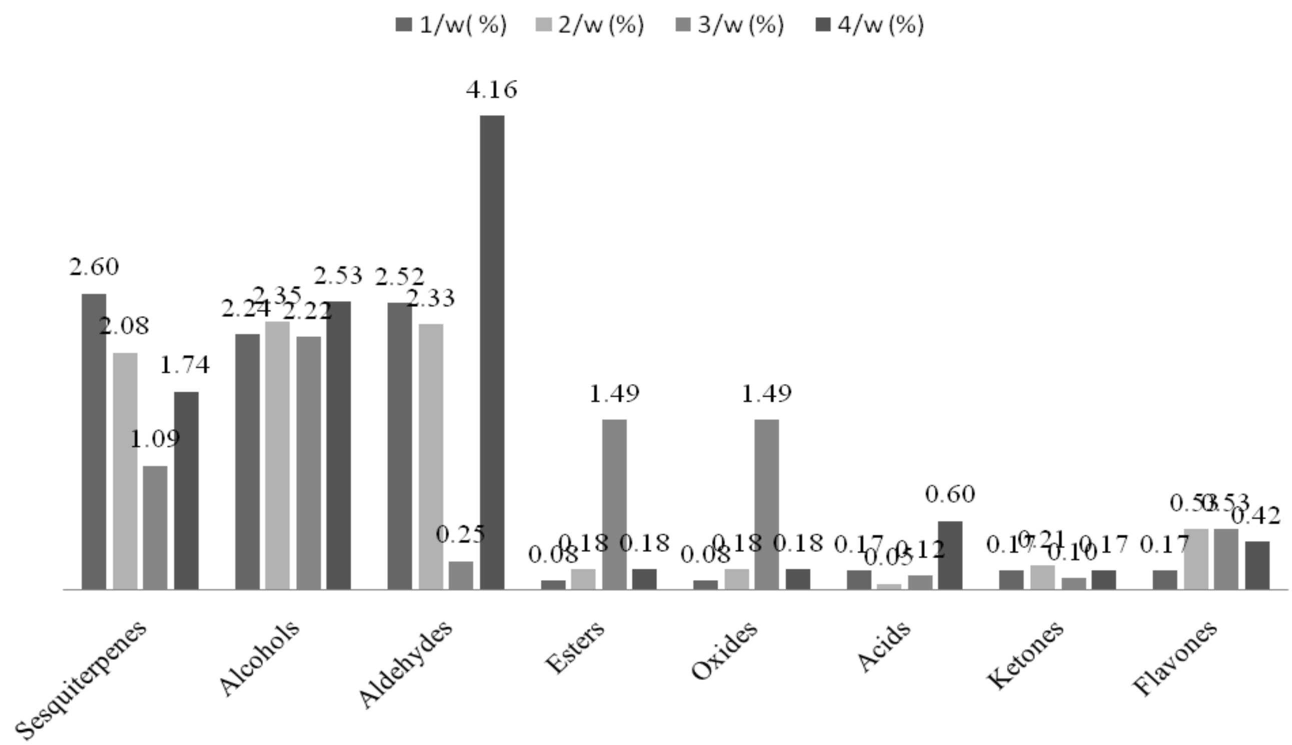

Fig: 2. Volatile composition of cold pressed mandarin oils expressed in (%)

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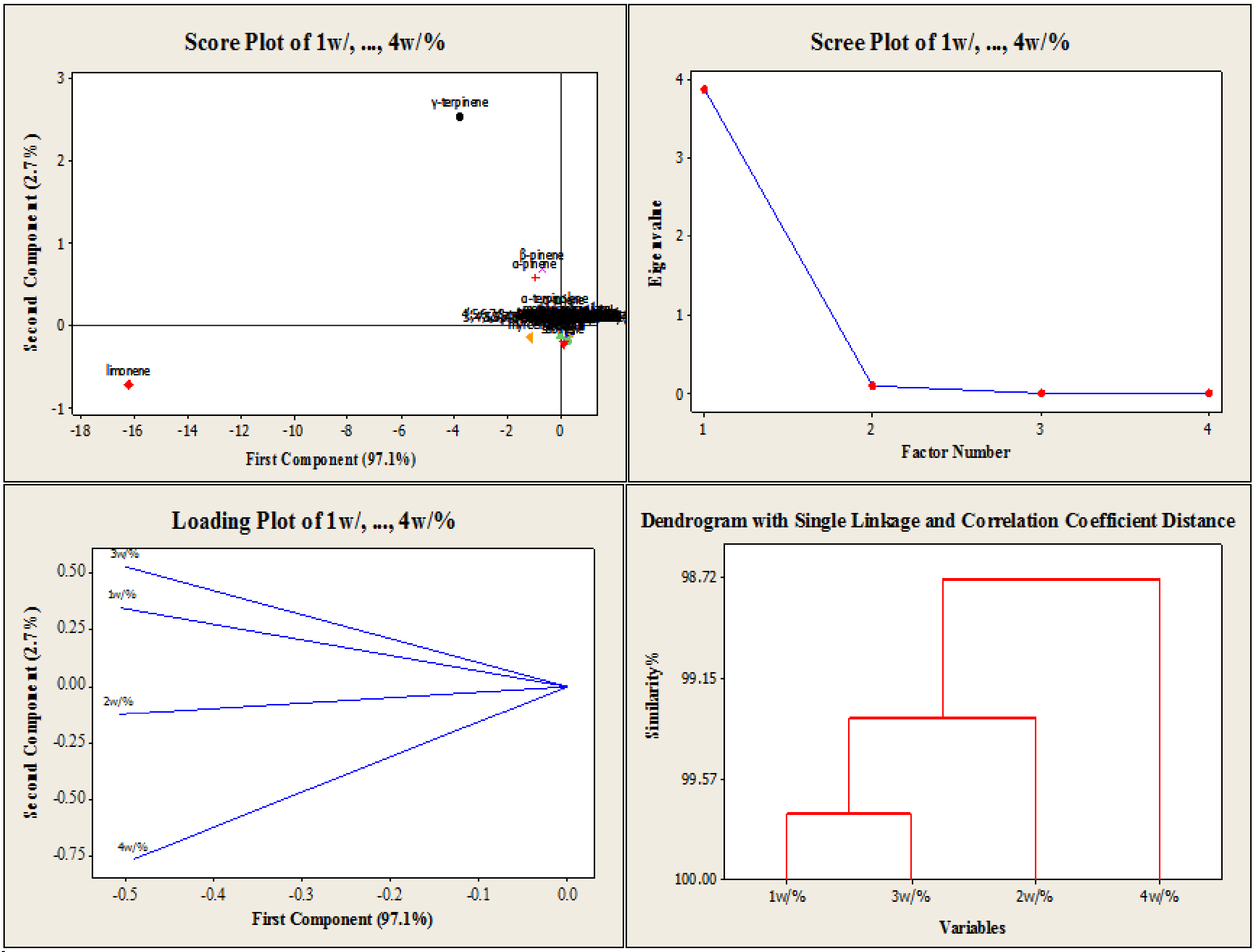

Fig: 3. PCA scatter plots and cluster dendrograms discriminating cold pressed mandarin oils and their volatile flavour compositions into different classes.

Except for some monoterpene hydrocarbons namely α-pinene, β-pinene, limonene and γ-terpinene, the other target volatile compounds could be classified in one group in PC1, because the coefficients of these volatile compounds were the same negative sign located in PC 1 **[Figure– 3]**. In most cases, the differentiation or closeness between the volatile flavour compounds directed in negative side of PC 1 was dependent on their chemical classes. The second principal component (PC 2) accounted for very small proportion (2.7%) of the total variability. As shown in **Figure– 3**, most of target volatile flavour compounds identified in cold pressed lemon oils namely alcohol (i.e. linalool, terpinen-4-ol, α-terpineol and geraniol), ester compounds (i.e. citronellyl acetate, neryl acetate and geranyl acetate) and aldehyde compounds (i.e. octanal decanal, citronellal, nonanal, neral and geranial) were classified with the same negative sign in PC 2; while α-pinene, β-pinene and γ-terpinene were placed in the positive side of PC 2 **[Figure– 3]**. Limonene and γ-terpinene were separated from the other volatiles because their percentage was significantly higher in comparison to other volatile compounds. α-pinene and β-pinene were closer to other compounds on PCA score plot because their abundance were lower than the abundance of the limonene and γ-terpinene. PCA score plot significantly differentiated the cold pressed mandarin oils from each other **[Figure– 3]**. As it is notable from the loading plot, samples 1 and 3 were closer in comparison to the samples 2 and 4.

Finally, their similarity was confirmed in the dendrogram with single linkage and correlation coefficient distance. Samples of cold pressed mandarin oil from South Africa and red mandarin oil from unknown region were classified as the most similar. If we compare the percentage of the volatiles for samples 1 and 3 **[Supplementary Table-1]** we can see that those two samples had the most similar composition. Because all the samples have been processed with the same technology at the same season, quantitative differences in the essential oil compositions might be due to the genetic origin which belongs to the different variety.

[V] CONCLUSION

In the present study, high resolution gas chromatography (HRGC) equipped with mass spectrometer (MS) was employed for the qualitative and quantitative analyses of volatile flavour compounds of different varieties of cold pressed mandarin oils. Multivariate analysis techniques aided in the interpretation of chemical data obtained for volatile components of mandarin oils. Differences among individual components provided less useful information, mainly because there is often a wide variation in the volatile fraction composition from different samples of the same oils; since multivariate analysis involves variability of several or all of the compounds; it seems that the discrimination results were less affected by such variation. Although the same technology was applied to process the studied cold pressed mandarin oils, quantitative differences in the essential oil composition could be attributed to the different varieties. The samples of red mandarin oil from South Africa and red mandarin oils from unidentified region were grouped in the same cluster and clearly separated from the yellow and sweet "Murcot" variety of mandarin oil.

FINANCIAL DISCLOSURE

This work is not supported by any financial assistance.

CONFLICT OF INTERESTS

The authors declare that they have no conflicts of interest.

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SUPPLEMENTARY TABLE (As supplied by author)

Supplementary Table: 1. Volatile composition of cold pressed peel oils from red (1), yellow (2), red from South America (3) and sweet "Murcot" (4) mandarin expressed as percentage (%).

No.	Components	*LRI	1w/%	2w/%	3w/%	4w/%	Aroma descriptor
	Hydrocarbons						
	Monoterpenes						
1.	α-tujene	926	1.23	0.15	1.46	0.02	-
2.	α-pinene	932	4.61	2.09	7.20	2.78	sweet
3.	camphene	947	0.06	0.04	0.20	0.03	camphoraceous
4.	sabinene	973	0.50	1.86	0.00	1.70	-
5.	β-pinene	976	5.17	2.30	5.27	0.00	wet soil
6.	myrcene	992	5.91	4.52	3.13	7.15	warm
7.	α-terpinene	1024	0.43	0.18	0.26	0.13	lemony
8.	α-phelandrene	1005	0.00	0.00	0.11	0.00	-
9.	δ-3-carene	1010	0.00	0.28	0.10	0.00	-
10.	limonene	1033	46.91	56.60	46.71	74.29	fresh
11.	*trans*-iso-limonene	1073	0.05	0.00	0.00	0.01	-
12.	*trans*-β-ocimene	1054	0.36	0.41	0.11	0.12	-
13.	γ-terpinene	1063	17.31	12.59	19.97	0.17	lime-like
14.	α-terpinolene	1090	2.92	2.82	1.13	0.19	citrus
15.	δ-4-carene	1352	0.04	0.00	0.00	0.00	-
	Total terpenes		85.50	83.84	85.65	86.59	
	Sesquiterpene						
16.	δ-elemene	1559	0.03	0.03	0.00	0.00	-
17.	α-copaene	1377	0.17	0.19	0.07	0.24	-
18.	β-cubebene	1392	0.14	0.15	0.04	0.21	-
19.	β-elemene	1393	0.12	0.12	0.04	0.10	fruity
20.	*trans*-α-bergamotene	1438	0.24	0.00	0.01	0.00	-
21.	*trans*-β-caryophilene	1421	0.32	0.18	0.35	0.10	fresh
22.	α-humulene	1455	0.06	0.05	0.06	0.04	woody
23.	β-farnesene	1458	0.07	0.10	0.02	0.26	fruity
24.	α-amorphene	1478	0.02	0.02	0.01	0.00	-
25.	germancren-D	1482	0.12	0.14	0.00	0.13	
26.	aromadendrene	1489	0.02	0.00	0.00	0.00	
27.	byciclogermacrene	1498	0.00	0.03	0.00	0.04	

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28.	valencene	1494	0.08	0.13	0.00	0.08	woody
29.	α-selinene	1498	0.15	0.00	0.13	0.00	-
30.	α-farnecene	1509	0.00	0.00	0.30	0.21	-
31.	α-murolene	1502	0.03	0.00	0.00	0.05	
32.	*trans*-α-bisabolene	1545	0.04	0.08	0.00	0.00	dry
33.	β-bisabolene	1887	0.78	0.65	0.00	0.00	-
34.	δ-cadinene	1525	0.18	0.21	0.06	0.28	-
35.	germancren-B	1559	0.03	0.00	0.00	0.00	-
	Total sesquiterpenes		**2.60**	**2.08**	**1.09**	**1.74**	
	Alcohols						
36.	*p*-menta-*trans*-2,8-dien-1-ol	1124	0.09	0.09	0.11	0.10	-
37.	*cis*-sabinene hydrate	1070	0.05	0.03	0.04	0.02	-
38.	terpinene-4-ol	1179	0.18	0.08	0.14	0.00	woody
39.	α-terpineol	1193	0.43	0.21	0.87	0.32	floral
40.	linalool	1103	1.23	1.72	0.60	1.90	sweet
41.	*cis*-carveol	1224	0.09	0.12	0.31	0.08	-
42.	*trans*-carveol	1205	0.00	0.00	0.03	0.00	-
43.	thymol	1296	0.08	0.00	0.11	0.00	-
44.	elemol	1552	0.06	0.05	0.00	0.09	-
45.	nerolidol	1566	0.02	0.03	0.00	0.01	-
46.	spatulenol	1581	0.01	0.02	0.01	0.01	-
	Total alcohols		**2.24**	**2.35**	**2.22**	**2.53**	
	Aldehydes						
	Aliphatic						
47.	octanal	1004	0.00	0.36	0.00	1.32	-
48.	nonanal	1108	0.07	0.05	0.00	0.38	floral
49.	decanal	1207	0.39	0.43	0.07	1.28	marine
50.	tridecanal	1510	0.03	0.00	0.00	0.00	-
51.	tetradecanal	1614	0.00	0.00	0.00	0.29	-
52.	(E,E)-2,4-decadienal	1319	0.02	0.02	0.00	0.02	-
	Monoterpenic						
53.	neral	1243	0.19	0.16	0.00	0.09	lemony
54.	citronellal	1155	0.12	0.12	0.02	0.50	powerful floral
55.	geranial	1272	0.25	0.26	0.00	0.16	flowery, fruity
56.	undecanal	1308	0.00	0.00	0.00	0.12	-
57.	peryl aldehyde	1276	0.17	0.14	0.00	0.00	-
58.	β-sinensal	1700	0.19	0.00	0.00	0.00	-
59.	α-sinensal	1757	1.09	0.79	0.16	0.00	-
	Total aldehydes		**2.52**	**2.33**	**0.25**	**4.16**	

BIOCHEMISTRY

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Esters							
60.	octyl acetate	1214	0.00	0.00	0.00	0.05	-
61.	methyl antranilate	1343	0.24	0.35	1.03	0.00	-
62.	citronelyl acetate	1355	0.05	0.05	0.08	0.13	rosy
63.	neryl acetate	1367	0.23	0.27	0.02	0.20	very sweet
64.	geranyl acetate	1385	0.11	0.08	0.04	0.04	dry
Total esters			**0.63**	**0.75**	**1.17**	**0.42**	
Oxides							
65.	cis-limonene oxide	1135	0.10	0.07	0.44	0.09	citrus like
66.	trans-limonene oxide	1139	0.07	0.09	0.61	0.07	citrus like
67.	cariophylene oxide	1586	0.01	0.02	0.44	0.02	woody
Total oxides			**0.08**	**0.18**	**1.49**	**0.18**	
Acids							
68.	Octanoic acide	1184	0.05	0.03	0.04	0.00	-
69.	Decanoic acide	1375	0.03	0.02	0.04	0.00	-
70.	Hexadecanoic acid	1876	0.09	0.00	0.04	0.01	-
Total acids			**0.17**	**0.05**	**0.12**	**0.01**	
Ketones							
71.	L-carvone	1246	0.15	0.19	0.10	0.17	-
72.	piperiton	1257	0.01	0.00	0.00	0.00	-
73.	nutcatone	1808	0.01	0.02	0.00	0.00	grapefruit
Total ketones			**0.17**	**0.21**	**0.10**	**0.17**	
Flavones							
74.	4’,5,6,7,8-pentamethoxy flavon (tangeretine)	-	0.17	0.09	0.25	0.00	-
75.	3,3’,4’,5,5’,7,8-heptamethoxy flavon	-	0.00	0.00	0.18	0.18	-
76	3’,4’,5,6,7,8-hexamethoxy flavon (nobiletin)	-	0.00	0.44	0.11	0.24	-
	Total flavones		**0.17**	**0.53**	**0.53**	**0.42**	

* Linear retention index obtained by GC-MS with HP-5 column.