Volume 6 Issue 2

## **Research Article**

# Chemical Composition Similarity Relationships among the Various Organs of the *Ilex cornuta* Lindl. & Paxton Based on the Analysis of Hydrophilic Volatile Compounds

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Received: March 31, 2021; Accepted: April 07, 2021; Published: April 10, 2021

## Abstract

In performing molecular profiling of secondary metabolites, a lot of research has focused on biogenic volatile organic compounds with medium to low polarity. In this study, chemical composition similarity relationships among the various organs of the *llex cornuta* Lindl. & Paxton were assessed based on the analysis of hydrophilic volatile compounds. GC-MS analysis was conducted to characterize and classify the chemical compounds. A total of 36, 46, 42, 25, 64, 26 compounds have been respectively extracted from the root, stem, stem skin, leaf, flower and fruit. The six organs have 3 common compounds and large percentages of exclusive compounds ranging from 36.0% to 62.5% with a mean of 49.8%, indicating substantial component differences among the different organs. The percentage of overlapping compounds between each of the two organs ranges from 10.9% to 44.0%, which is relatively small, further demonstrating the strong organ specificity of the chemical composition. The overlapping index is used to reveal the similarity among the organs. The stem shares the maximum similarity while the fruit the minimum similarity with the other organs. Aside from fruit, the average overlapping indices between each of the other two organs correlate well to their physical proximity. In conclusion, hydrophilic volatile metabolites are a class of natural products that are rarely investigated but constitute a significant part of the plant chemical composition. Chemical profiling of these metabolites could provide a valuable tool for the plant taxonomy and help understand the chemically mediated biological phenomena.

Keywords: Chemical composition similarity, GC-MS, Hydrophilic volatile compounds, Ilex cornuta Lindl. & Paxton, Plant taxonomy

## Introduction

Plant taxonomy is traditionally conducted based on macroscopic and microscopic morphological characteristics. Growing evidence suggests that many biologically relevant entities could be missed in the studies that rely solely on morphological traits, particularly since speciation is not always accompanied by morphological change [1,2]. In recent years, plant chemical taxonomy has been developed to perform classification based on a wide array of biologically active secondary metabolites [3]. The expression of secondary metabolites could vary due to convergent evolution or differential gene expression [4], suggesting that the metabolite content of plants may reveal more information on the bioactive pattern of plants in comparison to morphology characterization [5].

In performing molecular profiling of secondary metabolites, a lot of research has focused on biogenic volatile organic compounds with medium to low polarity [6-9]. Volatile compounds are secreted and part of them are volatilized immediately after secretion [10,11]. The remaining part is stored in the special structure of the plant as in the case of essential oils [12-14]. Additionally, Berlinck and collaborators found that the vast majority of new compounds from natural sources reported in recent literature are compounds of medium to low polarity. Water-soluble, volatile, minor and photosensitive natural products are yet poorly known. One of the possible reasons for this trend could be that organic solvents of medium to low polarity used in isolation procedures require less time and less sophisticated instrumentation to be evaporated [15]. The author speculates that there is a class of hydrophilic volatile compounds in plants that are dispersed or dissolved in the water phase, evaporated with water vapor, and whose polarity and volatility are somewhere between essential oils and watersoluble compounds. To protect this type of ingredients from loss during extraction, water vapor distillation is used to collect volatile compounds that are dispersed or dissolved in the plant's water phase. The root, stem, stem skin, leaf, flower and fruit of the Ilex cornuta Lindl. & Paxton were analyzed as study samples. Volatile essential oils were removed by using Soxhlet extraction method. Hydrophilic volatile compounds obtained by water reflux extraction are characterized and classified by quantitative GC-MS. The study revealed the potential use of hydrophilic volatile metabolites in the plant taxonomy and understanding the chemically mediated biological phenomena.

## Materials and Methods

### Material

*Ilex cornuta* Lindl. & Paxton was collected in Nanjing, China. Its roots, stems, stem skins, leaves, flowers and fruits were washed, cut into pieces, dried at 30°C and stored at 2-8°C prior to use.

### **Chemicals and Reagents**

Ethyl acetate was purchased from Xilong Chemical Co., Ltd (Shantou, China). Hexane was purchased from Shanghai Titan Scientific Co., Ltd (Shanghai, China). Activated carbon was purchased from Shanghai Chemical Reagent Procurement Center (Shanghai, China). C7-C40 saturated alkanes standard was purchased from Anpel Laboratory Technologies Inc. (Shanghai, China).

### **Sample Preparation**

Each sample was sliced and dried at 30°C. After ground into powder, the samples were sieved through 80 mesh followed by 180 mesh. Approximately 6 g of the sample were subjected to Soxhlet extractor method with hexane for 24 hrs to remove essential oils and other lipophilic compounds. The remainder was then removed and dried at 30°C in the ventilation cabinet. Approximately 4 g of the dried powder was then added into a 6 x 7 cm nonwoven bag together with three glass balls of 4 cm diameter. At least 3 segments of thread were used to separate and tighten the bag into 3 parts, each containing a glass ball and even amount of the dried powder. The bag was then placed in a flask and 2100 mL of water was subsequently added to soak the powder for about 2 hrs. After reflux extraction for 6 hrs, 2 L of distilled water was collected. The same reflux extraction was repeated to collect another 1 L of distilled water for a total of 3 L. After cooling, activated carbon (4 g) was added to absorb the active ingredients from the 3 L of distilled water for about 8 hrs. The activated carbon containing the active ingredients was then filtered and dried at 30°C for 12 hrs. Ethyl acetate was subsequently added to isolate the active ingredients from the activated carbon using Soxhlet extractor method for 8 hrs. The resulting ethyl acetate extract was left in the ventilation cabinet to dry at 30°C. The dried active ingredients were finally re-dissolved using ethyl acetate, filtrated through 0.22 µm filter and analyzed using GC-MS.

## **GC-MS** Analysis

Analysis of hydrophilic volatile compounds was performed using Shimadzu GCMS-QP2010 Single Quadrupole GC-MS (Kyoto, Japan). A Rxi-1 ms GC capillary column (30 cm length, 0.25 mm inner diameter and 0.25  $\mu$ m thick film) from Shimadzu (Kyoto, Japan) was used for analysis.

One microliter of sample was injected in split mode with split ratio of 5 to 1. GC inlet temperature is set at 280°C. High purity nitrogen ( $\geq$ 99.999%) was used as carrier gas in constant flow mode at 1 mL/min. The initial temperature of the GC oven is set at 60°C and held for 1 min, then ramped at 4°C/min to 160°C and held for 3 mins, followed by 2°C/min to 280°C and held for 6 mins. Finally, the temperature is raised to 300°C at 4°C/min and held for 6 mins. The mass spectrometer was operated in positive electron ionization mode at 70 eV and all spectra were recorded in full scan with a mass range of 40-700 Da. The interface temperature is set at 280°C and ion source temperature is set at 250°C.

### **Data Processing and Compound Identification**

The GC-MS data processing was done with Shimazdzu GCMS Solution software. Compound identification was performed by applying several assignments, e.g., reference standard analysis, retention index calculation, and by NIST08 Spectrum Library comparison. Only peaks with area greater than 3 million are analyzed. The overlapping percentage is calculated by the number of overlapping compounds divided by the total number of hydrophilic volatile compounds from each of the two organ and times 100. Overlapping index is calculated by the number of overlapping compounds squared and divided by the total number of hydrophilic volatile compounds from each of the two organs. In addition, hierarchical clustering analysis was performed with Python to assess the similarities between each of the two organs by analyzing the number of overlapping hydrophilic volatile compounds.

## **Results and Discussion**

The root, stem, stem skin, leaf, flower and fruit of the Ilex cornuta Lindl. & Paxton contain compounds that are water soluble and can volatilize with water vapor. These hydrophilic compounds do not separate from the water phase and possess greater polarity than essential oils. The largest number (64) of hydrophilic volatile compounds are isolated from the flower and the smallest (25) from the leaf, indicating that the number of hydrophilic volatile compounds varies greatly from organ to organ. The hydrophilic volatile compounds include aromatics, fatty acids, furans, heterocycle, esters, alkanes, ketones, halogens and other types of small molecular compounds. This is a diverse group of molecules that could contribute to the expression of biological information about the plant. Tables 1-6 present the lists of hydrophilic volatile compounds identified from the root, stem, stem skin, leaf, flower and fruit, respectively. The bold and italic fonts in the table are used to refer to exclusive compounds that are only found in the specific organ and not contained in any other organ.

As shown in Table 7, the total number of hydrophilic volatile compounds isolated from the six organs ranges from 25 to 64. There are 3 common compounds in the six organs, i.e. Dodecanoic acid, 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester and n-Hexadecanoic acid. This accounts for 12.0% of total hydrophilic volatile compounds for the leaf and 4.7% for the flower with an average of 8.4% for all the six organs, indicating the little commonality of the six organs. Each organ also has its exclusive compounds which are not found in any other organ. The percentage of exclusive compounds follows the order of flower > fruit > stem skin > root > stem > leaf. The flower has the largest number and percentage of the exclusive compounds, 40 and 62.5%, respectively. The leaf has the smallest number and percentage of the exclusive compounds, 9 and 36.0%, respectively. The stem and stem skin display medium numbers of exclusive compounds. The average percentage of the exclusive compounds in the six organs was 49.8%, nearly half, indicating strong organ specificity. These results provide evidence to support the

No	RT	RI	Compound	Formula
1	8.434	1041	2(3H)-Furanone, dihydro-4-hydroxy-	$C_4H_6O_3$
2	8.555	1044	2-Oxo-n-valeric acid	$C_5H_8O_3$
3	8.623	1047	2,3-Anhydro-d-galactosan	$C_6H_8O_4$
4	9.159	1064	Acetic acid, hexyl ester	$C_{8}H_{16}O_{2}$
5	9.767	1084	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-	$C_{7}H_{10}O_{2}$
6	12.753	1173	Octanoic Acid	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>
7	13.662	1199	2-Furancarboxaldehyde,5-(hydroxymethyl)-	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>
8	16.053	1269	Nonanoic acid	$C_{g}H_{18}O_{2}$
9	19.301	1364	Benzaldehyde, 4-(methylthio)-	$C_sH_sOS$
10	23.459	1492	1H-2-Benzopyran-1-one, 3,4-dihydro-8-hydroxy-3-methyl-	$C_{10}H_{10}O_{3}$
11	23.660	1498	3-Acetoxydodecane	$C_{14}H_{28}O_2$
12	25.161	1546	7-Hydroxy-3-(1,1-dimethylprop-2-enyl) coumarin	$C_{14}H_{14}O_{3}$
13	25.496	1557	Dodecanoic acid	C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>
14	25.696	1564	Estra-1,3,5(10)-trien-17. beta ol	$C_{18}H_{24}O$
15	26.109	1577	Butyric acid, 3-tridecyl ester	$C_{17}H_{34}O_{2}$
16	26.829	1600	Hexadecane	C <sub>16</sub> H <sub>34</sub>
17	27.305	1613	Ethanone, 1-[2-(5-hydroxy-1,1-dimethylhexyl)-3-methyl-2-cyclopropen-1-yl]-	C <sub>14</sub> H <sub>24</sub> O <sub>2</sub>
18	28.020	1631	Thieno[3,2-c]pyridin-4(5H)-one	C <sub>7</sub> H <sub>5</sub> NOS
19	28.671	1649	Dodecanoic acid, 3-hydroxy-	$C_{12}H_{24}O_{3}$
20	30.636	1700	2-Bromotetradecane	C <sub>14</sub> H <sub>29</sub> Br
21	32.780	1750	7-Methyl-Z-tetradecen-1-ol acetate	C <sub>17</sub> H <sub>32</sub> O <sub>2</sub>
22	35.860	1821	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>
23	37.894	1867	2a-isopropyl-9,10a-dimethyl-6-methylenedodecahydro-1H-cyclopenta[4',5']cycloocta[1',2':1,5] cyclopenta[1,2-b]oxiren-4-ol	C <sub>20</sub> H <sub>32</sub> O <sub>2</sub>
24	39.903	1912	1,2-Benzenedicarboxylic acid, butyl octyl ester	$C_{20}H_{30}O_4$
25	41.687	1951	n-Hexadecanoic acid	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>
26	49.181	2119	7-Hexadecenal, (Z)-	C <sub>16</sub> H <sub>30</sub> O
27	50.098	2139	9-Octadecenamide, (Z)-	$C_{18}H_{35}NO$
28	50.483	2148	Octadecanoic acid	C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>
29	59.601	2362	2-Methyloctadecan-7,8-diol	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>
30	65.148	2499	1,2-Benzenedicarboxylic acid, diisooctyl ester	$C_{24}H_{38}O_4$
31	73.761	2726	13-Docosenamide, (Z)-	C <sub>22</sub> H <sub>43</sub> NO
32	77.825	2840	3-Phenyl-2-ethoxypropylphthalimide	$C_{19}H_{19}NO_3$
33	83.874	3017	9,10-Secocholesta-5,7,10(19)-triene-3,24,25-triol, (3.beta.,5Z,7E)-	$C_{27}H_{44}O_3$
34	89.708	3197	Heptanoic acid, docosyl ester	C29H58O2
35	92.123	3265	Isophthalic acid, allyl pentadecyl ester	$C_{26}H_{40}O_4$
36	102.267	3561	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester	C <sub>35</sub> H <sub>62</sub> O <sub>3</sub>

Table 1: List of the hydrophilic volatile compounds identified from the root of the Ilex cornuta Lindl. & Paxton.

Note: The bold and italic fonts are used to refer to exclusive compounds. RT: Retention time. RI: Reflex index.

#### Table 2: List of the hydrophilic volatile compounds identified from the stem of the Ilex cornuta Lindl. & Paxton.

No	RT	RI	Compound	Molecular
1	13.608	1198	2-Furancarboxaldehyde, 5-(hydroxymethyl)-	$C_6H_6O_3$
2	19.258	1363	4-Hydroxy-2-methoxybenaldehyde	$C_8H_8O_3$
3	21.565	1433	Cyclopentanemethanol,.alpha(1-methylethyl)-2-nitro-, [1.alpha.(S*),2.alpha.]-	$C_{g}H_{I7}NO_{3}$
4	23.85	1504	4,8-Decadienal, 5,9-dimethyl-	$C_{12}H_{20}O$
5	24.743	1533	Megastigmatrienone	$C_{_{13}}H_{_{18}}O$

6025491558045704.0.1.0.1.0.1.0.1.0.1.0.0.1.0.0.0.0.0.0					
725.641570Protanois add, 2.24 irinardyl. 3.cnb.org/sapregl. tabalyt.eterC, H, O,826.051577Protanois add, 2.24 irinardyl. 3.cnb.org/sapregl. tabalyt.eterC, H, O,1026.051589P.Addryl.et. (2.6.6 irinardyl.5.3 cnb.org/sapregl. tabalyt.eter)C, H, O,1127.1771680Banadadyl.et. (Hydraws.).5.4 infinitolyt.eter)C, H, O,1227.781633Banadadyl.et. (Hydraws.).5.4 infinitolyt.eter)C, H, O,1327.881633G. Statulyt.eter)C, H, O,1424.771633G. Statulyt.eter)C, H, O,1524.771633G. Statulyt.eter)C, H, O,1624.771633G. P. P. P. Statulyt.eter.C, H, O,1724.971633G. P. P. P. Statulyt.eter.C, H, O,180.1971634G. P. P. P. Statulyt.eter.C, H, O,1919.091644Batanol, 1/23.3 irinarchyt.i (C. statulyt.eter.C, H, O,1930.411704Hatanos, 1/24.3 irinarchyt.i (C. statulyt.eter.C, H, O,1030.441704Batanos, 1/24.3 irinarchyt.i (C. statulyt.eter.C, H, O,1030.451775G. Batanos, 1/24.3 irinarchyt.i (C. statulyt.eter.C, H, O,1030.451774G. Batanos, 1/24.3 irinarchyt.i (C. statulyt.eter.C, H, O,1030.451774G. Batanos, 1/24.3 irinarchyt.i (C. statulyt.eter.C, H, O,1031.361774G. G. H, O,C, H, O,11 <td>6</td> <td>25.469</td> <td>1556</td> <td>Dodecanoic acid</td> <td><math>C_{12}H_{24}O_{2}</math></td>	6	25.469	1556	Dodecanoic acid	$C_{12}H_{24}O_{2}$
890.0051570Pertamics aid 2.24 rimsply 5 arbsylpappyliabely effect90.000982.05158010.0000.00010120.712710.000.0000.00011227.12710.000.0000.00011327.12710.000.0000.00011427.12710.000.0000.00011527.12710.000.0000.00011627.12710.000.0000.00011727.12710.000.0000.00011828.00010.0000.0000.00011928.00010.0000.0000.00011929.07010.0000.0000.00011929.07010.0000.0000.00011929.07010.0000.0000.00011929.07010.0000.0000.00011929.07010.0000.0000.00011929.07010.0000.0000.00011920.07010.0000.0000.00011920.07010.0000.0000.00011920.07010.0000.00000.000011920.00010.0000.00000.000011920.00010.00000.00000.000011920.00010.00000.00000.000011920.00010.00000.000000.0000011920.000010.000000.000000.00000<	7	25.681	1563	1-Cyclohexene-1-methanol, .alpha.,2,6,6-tetramethyl-	$C_{_{II}}H_{_{20}}O$
99XA35158116000160001600016000160001028.4881580158001600016000160001127.370164012banne, 1/2 (s) hybory, 1-4 interlyhyskyh 3-nehyl-2 cychopope, 1-yl:16000160001127.88164812banne, 1/2 (s) hybory, 1-4 interlyhyskyh 3-nehyl-2 cychopope, 1-yl:1600001600001227.88164912banne, 1/2 (s) hybory, 1-4 interlyhyskyh 3-nehyl-2 cychopope, 1-yl:1600001600001328.865164912banne, 1-2 (s) hybory, 1-4 interlyhyskyh 3-nehyl-2 (s) hybory, 1-4 interlyhyskyh 3-nehyl-2 (s) hybory, 1-4 interlyhyskyh 3-nehyl-1 (s) hybory, 1-	8	26.105	1577	Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester	$C_{16}H_{30}O_4$
1025.48515.892.Addyl.42.6.6.malyl.ychac.1-angl.in.2.a.1.a.dC. L. J. G.1127.12716.80Bazaládyka Alykovy.3-Sdunkovy.C. Q. L. Q.1227.2816.81Thanon 1.2.C. Mpory.1.1 dinnyt Mychyl.3-nethyl.2-cychopren 1.yll.C. Q. L. Q.1327.2816.82S. C. M. D.	9	26.245	1581	Phenol, 3,4,5-trimethoxy-	$C_9H_{12}O_4$
1110.7.121648Benaldshyd,-Hydroxy-S-S-dinethoxy.0.C.H.O.1210.7.1701640Bitanne,1,2 (Sphrynt). dimethylk-gr-barchylber).0.C.H.O.1320.2.8.2716480.7.115an(3.2.4.1yrchin.d.15).0.C.H.O.1440.2.8.2716490.7.115an(3.2.4.1yrchin.d.15).0.C.H.O.1550.2.8.6816490.7.115an(3.2.4.1yrchin.d.15).0.C.H.O.1660.2.1716490.7.115an(3.2.4.1yrchin.d.15).0.C.H.O.1760.3.2716490.7.115an(3.1.1yrchin.d.15).0.C.H.O.1780.3.2716490.7.115an(3.1.1yrchin.d.15).0.C.H.O.1790.3.3717090.7.115an(3.1.1yrchin.d.15).0.C.H.O.1700.3.1317170.7.115an(3.1.1yrchin.d.1yrchin.d.15).0.C.H.O.1700.3.1317180.7.115an(3.1yrchin.d.1yrchin	10	26.495	1589	2-Methyl-4-(2,6,6-trimethylcyclohex-1-enyl)-but-2-en-1-ol	$C_{14}H_{24}O$
11227371014Ithanas, 1/2 (s) hydnay, 1/, dimylhyl-), subhlyl-2, cyclopapen 1yl).C, l, l, o,1327381638GC, l/L, OC, l/L, O1427871638Spire (4.5) decar 7.ax, 1.8' dimylhyl-9, disyngyl-1.0C, l/L, O14278701649GC, l/L, OC, l/L, O1528.8581649GC, l/L, OC, l/L, O1629.0721642GC, l/L, OC, l/L, O1729.0711642GC, l/L, OC, l/L, O1830.3901690GC, l/L, OC, l/L, O1930.4901690GC, l/L, OC, l/L, O2030.4911700GC, l/L, OC, l/L, O2131.6701710GC, l/L, OC, l/L, O2331.6711720GC, l/L, OC, l/L, O2424.0521733GC, l/L, OC, l/L, O2531.751726GC, l/L, OC, l/L, O2631.831711GC, l/L, OC, l/L, O2731.831711GC, l/L, OC, l/L, O2831.841810GC, l/L, OC, l/L, O2931.841813GC, l/L, OC, l/L, O2031.841814GC, l/L, OC, l/L, O2131.841814GC, l/L, OC, l/L, O2131.841814GC, l/L, OC, l/L, O2131.841814GC, l/L, OC, l/L, O2131.841814GC, l/L, OC, l/L, O<	11	27.127	1608	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	$C_9H_{10}O_4$
14073804380439043904490140243704300507005.0%1502437046005.0%05.0%16024370046005.0%05.0%1702437046005.0%05.0%1803030046005.0%05.0%1903030040005.0%05.0%1003040040005.0%05.0%1003040040005.0%05.0%1003040040005.0%05.0%1003040040005.0%05.0%1003040040005.0%05.0%1003040040005.0%05.0%1003040040005.0%05.0%1003040040005.0%05.0%1003040040005.0%05.0%11040000400005.0%05.0%1203040040005.0%05.0%1304300040005.0%05.0%1404300040005.0%05.0%1504300040005.0%05.0%1604300040005.0%05.0%1604300040005.0%05.0%1604300040005.0%05.0%1604300040005.0%05.0%1604300040005.0%05.0%1704300040005.0%05.0%	12	27.37	1614	Ethanone, 1-[2-(5-hydroxy-1,1-dimethylhexyl)-3-methyl-2-cyclopropen-1-yl]-	$C_{14}H_{24}O_{2}$
14428271638Spire/4.51-scam?-one, 1.4 simulty1-8 sparsy-1-isopropy1-C, L, L, D,152868516492.8 mon dolcamC, L, B,162927716431.4 Phane, 2 condeclopacy)-C, L, L, D,162927116431.4 Phane, 2 condeclopacy)-sharementC, L, L, D,1730.3 Phane, 1 (2)1.6 Phane, 1 (2)C, L, L, D,1830.2 Phane, 1 (2)1.6 Phane, 1 (2)C, L, L, D,1930.3 Phane, 1 (2)1.6 Phane, 1 (2)C, L, L, D,2030.4 Phane, 1 (2)1.6 Phane, 2 (2)C, L, L, D,2131.4 Phane, 1 (2)1.7 Phane, 2 (2)C, L,	13	27.88	1628	Thieno[3,2-c]-pyridin-4(5H)-one	C <sub>7</sub> H <sub>5</sub> NOS
1 / / / / / / / / / / / / / / / / / / /	14	28.27	1638	Spiro-[4.5]-decan-7-one, 1,8-dimethyl-8,9-epoxy-4-isopropyl-	$C_{15}H_{24}O_2$
1 fet28/721/621/62Ethonol.2(oxtac)q(oxy)-C, L, Q,1728.97116.881.12.14/dray-4.5.4methory-phyn)-thomorC, L, Q,1830.30916.912.Popenul.3(4.14/dray)-smthory-phyn)-tychory-phyllC, L, Q,1830.30917.0010.001C, L, Q,101.30.0717.001.001C, L, Q,1231.03717.001.001C, C, L, Q,1231.03717.001.001C, C, L, Q,1231.03717.014.0101/backera, 2.0.1014-tertamethyl-C, C, L, Q,1231.03717.014.0101/backera, 2.0.1014-tertamethyl-C, C, L, Q,1231.03717.014.0101/backera, 2.0.1014-tertamethyl-C, C, L, Q,1231.32817.301.012C, C, L, Q,1231.32917.301.012C, C, L, Q,1331.32017.301.012C, L, Q,1431.32817.301.012C, L, Q,1531.32917.301.012C, L, Q,1631.3291.0121.012C, L, Q,1631.3291.0121.012C, L, Q,1531.3491.8131.012-1.8121.0121631.3491.8141.012-1.8121.0121731.3491.8141.012-1.8121.0121831.3991.8141.012-1.8121.0121931.3491.8141.012-1.8121.0121931.349	15	28.685	1649	2-Bromo dodecane	$C_{_{12}}H_{_{25}}Br$
112897116831/1/21/datay-4.5-dim datay-phenyl-rehanoneC_J_L_01830.0271169416943.0.2.2.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4	16	29.172	1662	Ethanol, 2-(octadecyloxy)-	$C_{_{20}}H_{_{42}}O_{_2}$
1890.27116911-2-Propend.3-(Alydray-3-methaxphenyl)-(C, μ, 0)1930.3991694Batanol,1-(2,2,3-stramethyl-1-(3-methyl-1-pennyl)-cyclopropyl)-(C, μ, 0)2030.0171700(Pathaccane C, 10)-(1-4-methyl-1-expanyl)-cyclopropyl)-(C, μ, 0)2131.0371717(Pathaccane C, A)-(1-4-ternmethyl-1-expanyl)-cyclopropyl)-(C, μ, 0)2231.1551716(Pathacone C, 10)-(1-4-ternmethyl-1-expan)(C, μ, 0)2331.0501713(Pathacone C, 10)-(1-4-ternmethyl-1-expan)(C, μ, 0)2432.0521713(Pathacone C, 10)-(1-4-ternmethyl-1-expan)(C, μ, 0)2532.7881719(C/clopropant, 1-(1-hydray-1-legpl)2-methylens-3-pentyl-(C, μ, 0)2632.831717(Pathacone C, 10)-(1-4-ternmethyl-1-expanyl-2-dimithylens-3-pentyl-(C, μ, 0)2733.6831813(Pathacone C, 10)-(1-4-ternmethyl-1-expanyl-2-dimithylens-3-pentyl-(C, μ, 0)2834.821800(Pathacone C, 10)-(1-4-ternmethyl-1-expanyl-2-dimithylens-3-pentyl-1-expansion-(C, μ, 0)2935.8691813(Pathacone C, 10)-(1-4-ternmethylens-1-expanyl-1-expansion-(C, μ, 0)3037.30118421840(Pathacone C, 10)-(1-4-ternmethylens-1-expansion-(C, μ, 0)3137.30518491941(Pathacone C, 10)-(1-4-ternmethylens-1-expansion-(C, μ, 0)3237.89818491942(Pathacone C, 10)-(1-4-ternethylens-1-expansion-(C, μ, 0)3339.907194214.01 <td< td=""><td>17</td><td>29.971</td><td>1683</td><td>1-(2-Hydroxy-4,5-dimethoxy-phenyl)-ethanone</td><td><math>C_{_{10}}H_{_{12}}O_{_4}</math></td></td<>	17	29.971	1683	1-(2-Hydroxy-4,5-dimethoxy-phenyl)-ethanone	$C_{_{10}}H_{_{12}}O_{_4}$
1930.3991644Batanol, 1-(22,3)-steramethyl-1-(3-methyl-1-persynl)-cyclopropril)-C, H, Q2030.6411700C, H, GC, H, G2131.0371710ICA Hendecane, 26,61,014-tetramethylC, H, G2231.0371710ICA Hendecane, 26,61,014-tetramethylC, H, G2331.751726ICA Mamatane, 1-thicoyantomethylC, C, H, S2432.0221733ICA IAC, C, H, O2532.521743ICA IAICA C, C, D2632.781750ICA IAICA IA2731.6831750ICA IAICA IA2832.7841780ICA IAICA IA2933.6831813ICA IAICA IA3053.5841813ICA IAICA IA3157.3161844ICA IAICA IA3157.31618492ISANICA IA, G3137.398189722ICA IA3139.9071912ICA IAICA IA, G3139.9071912ICA IAICA IA, G3139.9071912ICA IAICA IA, G3144.9171919ICA IAICA IA, G3119.90312.902ICA IAICA IA, G3219.90313.90ICA IAICA IA, G3339.90719.12ICA IAICA IA, G3449.90312.90ICA IAICA IA, G3543.89819.	18	30.271	1691	2-Propenal, 3-(4-hydroxy-3-methoxyphenyl)-	$C_{10}H_{10}O_3$
12030.6411700IPPROVEC_{B}_{L}21131.0371710GRADERAGEARA.2A.0A.14-tetrametyl-GR_B_A22233.1371712GRADERAGEARA.2A.0A.14-tetrametyl-GR_B_A23331.731720GRADERAGEARA.2A.0A.2A.8A.0A.9A.14.14.0A.2A.0A.2A.8A.0A.9A.14.14.0A.2A.0A.2A.9A.0A.14.14.0A.2A.0A.2A.0A.0A.14.0A.2A.0A.0A.14.0A.14.0A.2A.0A.2A.0A.14.0A.14.0A.2A.0A.14.0A.14.0A.2A.0A.14.0A.14.0A.2A.0A.14.0A.14.0A.2A.0A.14.0A.14.0A.2A.0A.14.0A.14.0A.2A.0A.14.0A.14.0A.2A.0A.14.0A.2A.0A.14.0A.14.0A.2A.0A.14.0A.14.0A.2A.0A.14.0A.14.0A.2A.0A.14.0A.14.0A.2A.0A.14.0A.14.0A.14.0A.14.0A.2A.0A.14.	19	30.399	1694	Butanol, 1-[2,2,3,3-tetramethyl-1-(3-methyl-1-penynyl)-cyclopropyl]-	$C_{17}H_{30}O$
11         31.037         17.10         Hexadcane, 2.6.10.14-termethyl- $C_{a}H_{a}$ 122         31.345         17.17 $Aa-Dichloromethyl-4.4a, 5.6.7.8-hexahydro-3H-naphthalen-2-one         C_{a}H_{a}Cl           123         31.75         17.26         Aa-Dichloromethyl-4.4a, 5.6.7.8-hexahydro-3H-naphthalen-2-one         C_{a}H_{a}Cl           124         32.052         17.33         Barchan A A A A A A A A A A A A A A A A A A A$	20	30.641	1700	Heptadecane	C <sub>17</sub> H <sub>36</sub>
22         31.345         1/17         4a-Dickloromethyl-4.4a.5.6.7.8-hexaltydro-3H-naphthalen-2-one $C_{\mu}H_{\mu}Cl_{\nu}O$ 23         31.75         1726         Adamantane, 1-thiocyanatomethyl- $C_{\alpha}H_{\nu}NS$ 24         32.052         1733         9-(3.3-Dimethylaxiran-2yl)-2.7-dimethylhom-2.6-dien-1-ol $C_{\alpha}H_{\nu}O_{\mu}$ 25         32.512         1744         1-Decanol, 2-bexyl- $C_{\alpha}H_{\nu}O$ 26         32.788         1750         Cyclopropane, 1-(1-hydraxy-1-heptyl)-2-adihydrop-spentyl- $C_{\alpha}H_{\nu}O$ 27         33.683         1771         3-bohutyr)-6-isopropyl-2.3-dihydrop-granz, 2-dione $C_{\nu}H_{\nu}O$ 28         3.4.92         1800         Heneixosane $C_{\nu}H_{\mu}$ 29         35.489         1813         Heptadecane, 2.6.10.15-tetramethyl- $C_{\alpha}H_{u}O$ 31         37.316         1854         1-1-Benzenedicarboxylic acid, bis(2-methylpropyl) ester $C_{\alpha}H_{u}O$ 33         39.907         1912         1.2-Benzenedicarboxylic acid, buyl 8-methylnonyl ester $C_{\nu}H_{u}O_{\mu}O_{\mu}O_{\mu}O_{\mu}O_{\mu}O_{\mu}O_{\mu}O_{\mu$	21	31.037	1710	Hexadecane, 2,6,10,14-tetramethyl-	$C_{20}H_{42}$
23         31.75         1726         Adamantane, 1-thiocyanatomethyl- $C_{n}H_{n}NS$ 24         32.052         1733         9-(3,3-Dimethylaxiran-2-yl)-2.7-dimethylnona-2.6-dien-1-ol $C_{n}H_{n}O_{1}$ 25         32.512         1744         1-Decanol, 2-hexyl- $C_{n}H_{n}O_{1}$ 26         32.2788         1750 $Cyclopropane, 1-(1-hydroxy-1-hetyl)-2methylne-3-pentyl-         C_{n}H_{n}O_{1}           27         33.680         1771         Cyclopropane, 1-(1-hydroxy-1-hetyl)-2methylne-3-pentyl-         C_{n}H_{n}O_{1}           28         34.92         1800         Heneicosane         C_{n,1}H_{n}O_{1}           30         35.86         1821         1-1-berzenedicarboxylic acid, bis(2-methylpropyl) ester         C_{n}H_{n,2}O_{1}           31         37.316         1854         1-1-berzenedicarboxylic acid, bis(2-methylpropyl) ester         C_{n}H_{n,2}O_{1}           33         39.907         1912         1.2-benzenedicarboxylic acid, hutyl 8-methylnoyl ester         C_{n}H_{n,0}O_{1}           34         41.693         1951         n-Hexadecanoi caid         C_{n}H_{n,0}O_{1}           35         43.899         2000         Ecosame         C_{n}H_{n,0}O_{1}           36         49.179         2119         12-Methyl-$	22	31.345	1717	4a-Dichloromethyl-4,4a,5,6,7,8-hexahydro-3H-naphthalen-2-one	$C_{_{11}}H_{_{14}}Cl_2O$
24         32.052         1733         9-(3,3-Dimethylaxiran-2-yl)-2.7-dimethylnona-2,6-dim-1-ol $C_{c}H_{a}O_{c}$ 25         32.512         1744         1-Decanol, 2-bexyl- $C_{c}H_{a}O$ 26         32.788         1750 $Cyclopropane, 1-(1-hydraxy-1-heptyl)-2-methylene-3-pentyl-         C_{c}H_{a}O           27         33.683         1771         Cyclopropane, 1-(1-hydraxy-1-heptyl)-2-methylene-3-pentyl-         C_{c}H_{a}O           28         34.92         1800         Cyclopropane, 1-(1-hydraxy-1-heptyl)-2-methylene3-pentyl-         C_{c}H_{a}O           29         33.683         1771         Stabotyryl-6-isopropl-2.3-dilhydropyran-2.4-dione         C_{c}H_{a}O           30         34.92         1800         Herptaceane, 2.6,10,15-terumethyle         C_{c}H_{a}O           31         37.848         1813         Herptaceane, 2.6,10,15-terumethyle         C_{a}H_{a}O           31         37.7346         1821         1.1-Benzenedicarboxylic aci,hulp-18eremethyle         C_{a}H_{a}O           32         37.898         1867         2^{1-sopropl-9,10a-dimethyl-6-methylendodecahydro-1H-cyclopenta[4:5]-cycloocta[1:2:1,5]-cyclopenta         C_{a}H_{a}O_{a}O           33         39.907         1912         1.2-Benzenedicarboxylic aci,d hulp-18eremethylonylester         C_{a}H_{a}$	23	31.75	1726	Adamantane, 1-thiocyanatomethyl-	C <sub>12</sub> H <sub>17</sub> NS
25         33.512         1744         International Probability Probabilit	24	32.052	1733	9-(3,3-Dimethyloxiran-2-yl)-2,7-dimethylnona-2,6-dien-1-ol	$C_{15}H_{26}O_{2}$
26         32.788         1750 $C_{cl} l_{so} 0$ 27         33.683         1771 $3.leobutyr)l-6.isoprop)l-2.3-dihydropyran-2.4-dione         C_{cl} H_{a} O_{l}           28         34.92         1800         1600         C_{cl} H_{a} O_{l}           29         35.489         1813         1710         C_{cl} H_{a} O_{l}           30         35.86         1821         1.12-Benzenedicarboxylic acid, bis(2-methylpropyl) ester         C_{cl} H_{a} O_{l}           31         37.316         1854         1.12-Benzenedicarboxylic acid, bis(2-methylpropyl) ester         C_{cl} H_{a} O_{l}           32         37.898         1867         2-isopropyl-9.10a-dimethyl-6-methylenedodcalydro-1H-cyclopenta[4,5]-cycloocta[1,2:1,5]-cycloopenta[4,5]         C_{cl} H_{a} O_{l}           33         39.907         1912         1.2-Benzenedicarboxylic acid, butyl 8-methylnonyl ester         C_{cl} H_{a} O_{l}           34         41.693         1951         n-Hexadecanoic acid         C_{cl} H_{a} O_{l}           35         43.899         2000         C_{cl} H_{a} O_{cl} C_{cl} H_{a} O_{l}           37         50.464         2148         Octadecanoic acid         C_{cl} H_{a} O_{l}           38         59.603         2562         2499         1.2-Benzenedicarbox$	25	32.512	1744	1-Decanol, 2-hexyl-	$C_{16}H_{34}O$
$27$ $33.683$ $1771$ $3-lsobutyrl-6-isopropl-2,3-dihydropran-2,4-dione         C_{c}H_{a}O_{c} 28 34.92 1800 1000 C_{n}H_{ai} 29 35.489 1813 Intericosane C_{n}H_{ai} 30 55.86 1821 Intericosane C_{n}H_{ai}O_{c} 31 37.316 1854 Intericosane C_{n}H_{ai}O_{c} 31 37.316 1854 Intericosane C_{n}H_{ai}O_{c} 32 37.898 1867 a^{isopropl-9,10a-dimethyl-emethyleedodeclaydydro-H-eyclopental(1, 2): 1,51-cyclopental         C_{n}H_{a}O_{c}O_{c} 33 39.907 1912 Intericosane C_{n}H_{n}O_{c}O_{c} 34 41.693 1951 Intericosane C_{n}H_{n}O_{c}O_{c} 35 43.899 2000 Intericosane C_{n}H_{n}O_{c}O_{c}H_{n}O_{c}O_{c} 37 50.464 2148 Ottadecanoic acid         C_{n}H_{n}O_{c}O_{c}H_{n}O_{c}O_{c}H_{n}O_{c}O_{c}H_{n}O_{c}O_{c}H_{n}O_{c}O_{c}H_{n}O_{c}O_{c}H_{n}O_{c}O_{c}H_{n}O_{c}O_{c}H_{n}O_{c}O_{c}H_{n}O_{c}O_{c}H_{n}O_{c}O_{c}H_{n}O_{c}O_{c}H_{n}O_{c}O_{c}H_$	26	32.788	1750	Cyclopropane, 1-(1-hydroxy-1-heptyl)-2-methylene-3-pentyl-	$C_{16}H_{30}O$
28         34.92         1800         Hencicosane $C_{\alpha}H_{sc}$ 29         35.489         1813         Interplatecane, 2,6,10,15-tertamethyl- $C_{\alpha}H_{sc}$ 30         35.86         1821         Interplatecane, 2,6,10,15-tertamethyl-popyl)ester $C_{\alpha}H_{sc}O_{s}$ 31         37,316         1854         Interplatecane, 2,6,10,15-tertamethyl-popyl)ester $C_{\alpha}H_{sc}O_{s}$ 32         37,316         1854         Interplatecane, 2,6,0,0,114-cyclopenta[4,57]-cyclootent1/2,21,5]-cyclopenta[4,57] $C_{\alpha}H_{sc}O_{s}$ 33         39,907         1912         interplatedicarboxylic acid, butyl 8-methylnonyl ester $C_{\alpha}L_{s,0}Q_{s}$ 34         44.693         1951         Interplatecane, 2,0,0 $C_{\alpha}L_{s,0}Q_{s}$ 35         43.899         2000         Interplatecane, 2,0,0 $C_{\alpha}L_{s,0}Q_{s}$ 36         44.1693         1951         Interplatecane, 2,0,0 $C_{\alpha}L_{s,0}Q_{s}$ 37         50.464         2148         Interplatecane, 2,0,0 $C_{\alpha}L_{s,0}Q_{s}$ 38         59.603         262         Interplatecane, 2,0,0 $C_{\alpha}L_{s,0}Q_{s}$ 39         65.152         2499         Interplatecane, 2,0,0 $C_{\alpha}L$	27	33.683	1771	3-Isobutyryl-6-isopropyl-2,3-dihydropyran-2,4-dione	$C_{_{12}}H_{_{16}}O_{_4}$
2935.891813Heptadecane, 2,6,10,15-tetramethyl- $C_{n}H_{4}$ 3035.8618211.12-Benzenedicarboxylic acid, bis(2-methylpropyl) ester $C_{k}H_{2}O_{k}$ 3137.31618541854 $C_{k}H_{1}O_{k}$ 3237.8981867 $2^{isispropyl-9,10a-dimethyl-6-methylenedodecahydro:1H-cyclopenta[4,5]-cycloocta[1,2:1,5]-cyclopentaC_{k}M_{2}O_{k}3339.90719121.12-Bioxiren-4-olC_{k}M_{2}O_{k}3441.6931951C_{k}M_{2}O_{k}C_{k}M_{2}O_{k}3543.8992000C_{k}M_{k}O_{k}C_{k}M_{k}O_{k}3649.17921191.2-Methyl-E,E,2,13-octadecahien-1-olC_{k}M_{k}O_{k}3750.4642148C_{k}M_{k}O_{k}C_{k}M_{k}O_{k}3859.60323622.4OCT_{k}M_{k}O_{k}C_{k}M_{k}O_{k}4073.75727261.2-Bioxienedicarboxylic acid, diisooctyl esterC_{k}M_{k}O_{k}4183.8613016C_{k}M_{k}O_{k}C_{k}M_{k}O_{k}4289.71131971.7(.5-Dimethylhexyl)-10.13-dimethyl-3-styrylhexadecahydrocylcapenta[a]phenanthren-2-oneC_{k}M_{k}O_{k}4492.6632801.7(.1,5-Dimethylhexyl)-10.13-dimethyl-14-tydroxy-, octadecyl esterC_{k}M_{k}O_{k}4594.57133314.Nortanosta-17(O),24-diene-11,16-diol-21-oic acid, 3-son-16.21-lactonC_{k}M_{k}O_{k}4610.22633561Benzenerpropanoic acid, 3.5-bis(1,1-dimethyl-4-tydroxy-, octadecyl esterC_{k}M_{k}O_{k}$	28	34.92	1800	Heneicosane	$C_{_{21}}H_{_{44}}$
30         3586         1821         1.2-Benzendicarboxylic acid, bis(2-methylpropyl) ester $C_{in} H_{2}, O_{1}$ 31         37.316         1854         1 $C_{in} H_{2}, O_{1}$ 32         37.898         1867 $2a$ -isopropyl-9,10a-dimethyl-6-methylenedodecahydro-1H-cyclopenta[4',5']-cycloocta[1',2:1,5]-cycloopta] $C_{2n} H_{2}, O_{1}$ 33         39.907         1912 $1.2-Benzenedicarboxylic acid, butyl 8-methylonoyl ester         C_{2n} H_{2}, O_{1}           34         41.693         1951         1.2-Benzenedicarboxylic acid, butyl 8-methylonoyl ester         C_{2n} H_{2}, O_{1}           35         43.899         2000         1.2-Benzenedicarboxylic acid, butyl 8-methylonoyl ester         C_{2n} H_{2}, O_{1}           36         49.179         2119         1.2-Benzenedicarboxylic acid, butyl 8-methylonoyl ester         C_{2n} H_{2n}, O_{1}           37         50.464         2148         0.000 C_{2n} H_{2n}, O_{1} C_{2n} H_{2n}, O_{1}           38         59.603         2362         0.0000 C_{2n} H_{2n}, O_{1} C_{2n} H_{2n}, O_{2n}           39         65.152         2499         0.0000 C_{2n} H_{2n}, O_{1} C_{2n} H_{2n}, O_{2n}           41         83.861         3016         0.000$	29	35.489	1813	Heptadecane, 2,6,10,15-tetramethyl-	$C_{21}H_{44}$
31         37.316         1854         Internation $C_{16}H_{3}O$ 32         37.898         1867         2*isopropl-9,10a-dimethyl-6-methylenedodecahydro-1H-cyclopenta[4,5]-cycloocta[1/2':1,5]-cycloot $C_{20}H_{30}O$ 33         39.907         1912         1122 $C_{20}H_{30}O$ 34         41.693         1951 $C_{20}H_{10}O$ $C_{20}H_{30}O$ 35         43.899         2000 $C_{10}O = 0$ $C_{20}H_{20}O = 0$ 36         49.179         2119 $C_{10}O = 0$ $C_{20}H_{30}O = 0$ 37         50.464         2148 $C_{10}O = 0$ $C_{10}H_{30}O = 0$ 37         50.464         2148 $C_{10}O = 0$ $C_{10}H_{30}O = 0$ 38         59.603         2362 $C_{10}O = 0$ $C_{10}H_{30}O = 0$ 39         65.152         2499 $C_{10}O = 0$ $C_{20}H_{30}O = 0$ 41         83.861         3016 $C_{20}H_{30}O = 0$ $C_{20}H_{30}O = 0$ 42         89.711         3197 $C_{10}O = 0$ $C_{20}H_{30}O = 0$ 43         92.16         3260 $17.(1,5-Dimethylexyl)-10,13-dimethyl-3-styrylhxadecahydrox$	30	35.86	1821	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	$C_{16}H_{22}O_4$
32         37.898         1867         2-isopropl-9,10a-dimethyl-6-methylenedodecahydro-1H-cyclopenta[4,5]-cycloocta[1,2:1,5]-cyclopenta $C_{20}H_{32}O_{2}$ 33         39.907         1912         1.12-Binzrenedicarboxylic acid, butyl 8-methylnonyl ester $C_{20}H_{32}O_{2}$ 34         41.693         1951 $C_{10}H_{20}O_{2}$ $C_{10}H_{20}O_{2}$ 35         43.899         2000 $C_{10}H_{20}O_{2}$ $C_{10}H_{20}O_{2}$ 36         49.179         2119 $C_{10}H_{20}O_{1}$ $C_{10}H_{30}O_{1}$ 37         50.464         2148 $C_{10}H_{30}O_{1}$ $C_{10}H_{30}O_{1}$ 38         59.603         2362 $C_{20}H_{20}O_{1}$ $C_{21}H_{30}O_{1}$ 39         65.152         2499 $C_{10}O_{1}$ $C_{21}H_{30}O_{1}$ 41         83.861         3016 $C_{21}H_{30}O_{1}$ $C_{21}H_{30}O_{1}$ 42         89.711         3197 $C_{20}O_{1}$ $C_{20}H_{40}O_{1}$ 43         92.16         3260 $17.(1,5-Dimethylhexyl-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[a]phenanthren-2-one         C_{20}H_{40}O_{1}           44         92.66         3280         17.(1,5-Dimethylhexyl-10,13-dimeth$	31	37.316	1854	1-Hexadecanol	$C_{16}H_{34}O$
33         39.907         1912         1,2-Benzenedicarboxylic acid, butyl 8-methylnonyl ester $C_{2}H_{3}O_{4}$ 34         41.693         1951 $n$ -Hexadecanoic acid $C_{16}H_{20}O_{2}$ 35         43.899         2000 $C_{00}H_{42}$ $C_{00}H_{42}$ 36         49.179         2119 $C_{10}H_{20}O_{10}$ $C_{10}H_{20}O_{10}$ 37         50.464         2148 $C_{10}H_{20}O_{10}$ $C_{10}H_{20}O_{10}$ 38         59.603         2362 $C_{2}OHthyloctadecan-7,8-diol         C_{10}H_{40}O_{2}           39         65.152         2499         1.2-Benzenedicarboxylic acid, diisooctyl ester         C_{22}H_{30}O_{3}           40         73.757         2726         13-Docosenamide, (Z)-         C_{22}H_{30}NO           41         83.861         3016         C_{22}H_{30}O_{3} C_{22}H_{30}O_{3}           42         89.711         3197         C_{20}H_{20}O_{11} C_{20}H_{30}O_{3}           43         92.16         3260         17-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[a]phenanthren-2-one         C_{20}H_{30}O_{3}           44         92.66         3280         17-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocycl$	32	37.898	1867	2a-isopropyl-9,10a-dimethyl-6-methylenedodecahydro-1H-cyclopenta[4',5']-cycloocta[1',2':1,5]-cyclopenta- [1,2-b]oxiren-4-ol	$C_{20}H_{32}O_{2}$
$34$ $41.693$ $1951$ $n$ -Hexadecanoic acid $C_{1s}H_{30}O_{2}$ $35$ $43.899$ $2000$ $2000$ $Eicosane$ $C_{3y}H_{42}$ $36$ $49.179$ $2119$ $12-Methyl-E,E-2,13-octadecadien-1-ol$ $C_{1y}H_{x0}O_{2}$ $37$ $50.464$ $2148$ $Octadecanoic acidC_{1s}H_{x0}O_{2}3859.60323622162C_{1y}H_{0}O_{2}3965.15224991.2-Benzenedicarboxylic acid, diisooctyl esterC_{2s}H_{3s}O_{4}4073.7572726C_{10}Chillip iso-allocholateC_{2s}H_{4}O_{5}4183.8613016C_{10}Chillip iso-allocholateC_{2s}H_{4}O_{5}4289.7113197Ir(-1,5-Dimethylhexyl-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[alphenanthren-2-one]C_{2s}H_{40}O_{4}4492.663280Ir(-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[alphenanthren-2-one]C_{2s}H_{40}O_{4}46102.2633561Benzenepropanoic acid, 3.5-bis(1,1-dimethylheyh)-4-hydroxy-, octadecyl esterC_{2s}H_{40}O_{4}$	33	39.907	1912	1,2-Benzenedicarboxylic acid, butyl 8-methylnonyl ester	$C_{22}H_{34}O_4$
$35$ $43.899$ $2000$ $Eicosane$ $C_{2x}H_{42}$ $36$ $49.179$ $2119$ $2119$ $12-Methyl-E,E-2,13-octadecadien-1-ol$ $C_{1y}H_{x0}O$ $37$ $50.464$ $2148$ $Octadecanoic acidC_{1y}H_{x0}O_23859.60323622000C_{1y}H_{40}O_23965.15224991.2-Benzenedicarboxylic acid, diisooctyl esterC_{2x}H_{3x}O_44073.7572726Octadecanoic acidC_{2x}H_{40}O_34183.8613016C_{2x}H_{40}O_3C_{2x}H_{40}O_34289.7113197Octadecanoic acid, docosyl esterC_{2x}H_{40}O_44392.16326017-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[a]phenanthren-2-oneC_{2x}H_{40}O_44492.66328017-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[a]phenanthren-2-oneC_{2x}H_{40}O_44594.57133314-Norlanosta-17(20),24-diene-11,16-diol-21-oic acid, 3-cox-16,21-lactoneC_{2x}H_{40}O_446102.2633561Benzenepropanoic acid, 3,5-bis(1,1-dimethyl-4-hydroxy-, octadecyl esterC_{x}H_{x}O_{x}$	34	41.693	1951	n-Hexadecanoic acid	$C_{16}H_{32}O_{2}$
$36$ $49.179$ $2119$ $12-Methyl-E,E,2,13-octadecadien-1-ol$ $C_{\mu_3}H_{s_0}O$ $37$ $50.464$ $2148$ $2148$ $C_{11}H_{10}O_2$ $38$ $59.603$ $2362$ $2362$ $C_{1.2}-Methyloctadecan-7,8-diolC_{1.2}H_{s_0}O_23965.15224991.2-Benzenedicarboxylic acid, diisooctyl esterC_{2.2}H_{3.0}O_44073.7572726C_{2.2}H_{3.0}O_1C_{2.2}H_{3.0}O_24183.8613016C_{2.2}H_{4.0}O_2C_{2.2}H_{4.0}O_24289.7113197P_{10}C_{2.0}H_{2.0}O_14392.16326617-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[a]phenanthren-2-oneC_{2.0}H_{4.0}O_14492.6633314-Norlanosta-17(20),24-diene-11,16-diol-21-oic acid, 3-oxo-16,21-lactoneC_{2.9}H_{4.0}O_146102.2633561Benzenepropanoic acid, 3,5-bis(1,1-dimethyl-4-hydroxy-, octadecyl esterC_{,H_{c.}O_{1}}$	35	43.899	2000	Eicosane	$C_{20}H_{42}$
37         50.464         2148         Octadecanoic acid         C <sub>18</sub> H <sub>36</sub> O <sub>2</sub> 38         59.603         2362         C	36	49.179	2119	12-Methyl-E,E-2,13-octadecadien-1-ol	$C_{_{I9}}H_{_{36}}O$
38         59.603         2362         2-Methyloctadecan-7,8-diol $C_{19}H_{40}O_2$ 39         65.152         2499         1,2-Benzenedicarboxylic acid, diisooctyl ester $C_{24}H_{38}O_4$ 40         73.757         2726 $C_{21}H_{30}O_2$ $C_{22}H_{40}NO$ 41         83.861         3016 $C_{26}H_{44}O_5$ $C_{29}H_{40}O_5$ 42         89.711         3197         Heptanoic acid, docosyl ester $C_{29}H_{30}O_4$ 43         92.16         3266         Isophthalic acid, allyl pentadecyl ester $C_{26}H_{40}O_4$ 44         92.66         3280         17-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[a]phenanthren-2-one $C_{29}H_{42}O_4$ 45         94.571         3331         4-Norlanosta-17(20),24-diene-11,16-diol-21-oic acid, 3-oxo-16,21-lactone $C_{29}H_{42}O_4$	37	50.464	2148	Octadecanoic acid	$C_{18}H_{36}O_{2}$
3965.15224991,2-Benzenedicarboxylic acid, diisooctyl ester $C_{24}H_{38}O_4$ 4073.757272613-Docosenamide, (Z)- $C_{21}H_{40}NO$ 4183.8613016C_{26}H_{40}O_5 $C_{26}H_{40}O_5$ 4289.7113197Model and the petanoic acid, docosyl ester $C_{29}H_{58}O_2$ 4392.16326617-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[a]phenanthren-2-one $C_{35}H_{52}O$ 4594.57133314-Norlanosta-17(20),24-diene-11,16-diol-21-oic acid, 3-oxo-16,21-lactone $C_{29}H_{42}O_4$ 46102.2633561Benzenepropanoic acid, 3,5-bis(1,1-dimethyl)-4-hydroxy-, octadecyl ester $C_{2,1}H_{2,0}O_4$	38	59.603	2362	2-Methyloctadecan-7,8-diol	$C_{19}H_{40}O_2$
4073.757272613-Docosenamide, (Z)- $C_{22}H_{43}NO$ 4183.8613016Ethyl iso-allocholate $C_{26}H_{44}O_5$ 4289.7113197Heptanoic acid, docosyl ester $C_{29}H_{58}O_2$ 4392.163266Isophthalic acid, allyl pentadecyl ester $C_{26}H_{40}O_4$ 4492.66328017-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[a]phenanthren-2-one $C_{25}H_{52}O$ 4594.57133314-Norlanosta-17(20),24-diene-11,16-diol-21-oic acid, 3-oxo-16,21-lactone $C_{27}H_{42}O_4$ 46102.2633561Benzenepropanoic acid, 3,5-bis(1,1-dimethyl)-4-hydroxy-, octadecyl ester $C_{12}H_{-1}O_1$	39	65.152	2499	1,2-Benzenedicarboxylic acid, diisooctyl ester	$C_{24}H_{38}O_4$
41         83.861         3016         Ethyl iso-allocholate $C_{2,b}H_{44}O_5$ 42         89.711         3197         Heptanoic acid, docosyl ester $C_{2,y}H_{3,s}O_2$ 43         92.16         3266         Isophthalic acid, allyl pentadecyl ester $C_{2,s}H_{40}O_4$ 44         92.66         3280         17-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[a]phenanthren-2-one $C_{3,s}H_{5,2}O$ 45         94.571         3331         4-Norlanosta-17(20),24-diene-11,16-diol-21-oic acid, 3-oxo-16,21-lactone $C_{2,y}H_{4,2}O_4$ 46         102.263         3561         Benzenepropanoic acid, 3,5-bis(1,1-dimethyl)-4-hydroxy-, octadecyl ester $C_{1,z}H_{-x}O_1$	40	73.757	2726	13-Docosenamide, (Z)-	C <sub>22</sub> H <sub>43</sub> NO
42         89.711         3197         Heptanoic acid, docosyl ester $C_{29}H_{38}O_2$ 43         92.16         3266         Isophthalic acid, allyl pentadecyl ester $C_{26}H_{40}O_4$ 44         92.66         3280         17-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[a]phenanthren-2-one $C_{35}H_{52}O$ 45         94.571         3331         4-Norlanosta-17(20),24-diene-11,16-diol-21-oic acid, 3-oxo-16,21-lactone $C_{29}H_{42}O_4$ 46         102.263         3561         Benzenepropanoic acid, 3,5-bis(1,1-dimethyl)ethyl)-4-hydroxy-, octadecyl ester $C_{12}H_{-1}O_1$	41	83.861	3016	Ethyl iso-allocholate	$C_{26}H_{44}O_5$
4392.163266Isophthalic acid, allyl pentadecyl ester $C_{2b}H_{40}O_4$ 4492.66328017-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[a]phenanthren-2-one $C_{35}H_{52}O$ 4594.57133314-Norlanosta-17(20),24-diene-11,16-diol-21-oic acid, 3-oxo-16,21-lactone $C_{2y}H_{42}O_4$ 46102.2633561Benzenepropanoic acid, 3,5-bis(1,1-dimethyl)-4-hydroxy-, octadecyl ester $C_{12}H_{20}O_{11}$	42	89.711	3197	Heptanoic acid, docosyl ester	$C_{29}H_{58}O_{2}$
4492.66328017-(1,5-Dimethylhexyl)-10,13-dimethyl-3-styrylhexadecahydrocyclopenta[a]phenanthren-2-one $C_{_{35}}H_{_{52}}O$ 4594.57133314-Norlanosta-17(20),24-diene-11,16-diol-21-oic acid, 3-oxo-16,21-lactone $C_{_{29}}H_{_{42}}O_4$ 46102.2633561Benzenepropanoic acid, 3,5-bis(1,1-dimethyllethyl)-4-hydroxy-, octadecyl ester $C_{_{12}}H_{_{22}}O_4$	43	92.16	3266	Isophthalic acid, allyl pentadecyl ester	$C_{26}H_{40}O_4$
45         94.571         3331         4-Norlanosta-17(20),24-diene-11,16-diol-21-oic acid, 3-oxo-16,21-lactone $C_{2y}H_{42}O_4$ 46         102.263         3561         Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester $C_{1z}H_{z2}O_4$	44	92.66	3280	17-(1,5-Dimethyl hexyl)-10,13-dimethyl-3-styryl hexadeca hydrocyclopenta [a] phen anthren-2-one the styryl hexadeca hydrocyclopenta hydrocyc	$C_{35}H_{52}O$
46 102.263 3561 Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester C <sub>1z</sub> H <sub>c2</sub> O,	45	94.571	3331	4-Norlanosta-17(20),24-diene-11,16-diol-21-oic acid, 3-oxo-16,21-lactone	$C_{29}H_{42}O_4$
	46	102.263	3561	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester	C <sub>35</sub> H <sub>62</sub> O <sub>3</sub>

Note: The bold and italic fonts are used to refer to exclusive compounds. RT: Retention time. RI: Reflex index.

No	RT	RI	Compound	Molecular			
1	12.765	1173	Octanoic Acid	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>			
2	13.818	1204	2-Furancarboxaldehyde, 5-(hydroxymethyl)-	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>			
3	19.283	1364	Benzaldehyde, 3-hydroxy-4-methoxy-	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>			
4	21.526	1432	2H-Pyran-2-one, 5,6-dihydro-6-pentyl-	$C_{10}H_{16}O_{2}$			
5	23.372	1489	4,6-di-tert-Butyl-m-cresol	$C_{15}H_{24}O$			
6	23.599	1496	12-Oxa-[tetracyclo[5.2.1.1(2,6).1(8,11)]]dodecan-10-ol, 3-acetoxy-	$C_{13}H_{18}O_{4}$			
7	23.856	1504	2,6-Dimethoxybenzoquinone	$C_{g}H_{g}O_{4}$			
8	25.171	1547	1H-Benzocyclohepten-7-ol, 2,3,4,4a,5,6,7,8-octahydro-1,1,4a,7-tetramethyl-, cis-	$C_{15}H_{26}O$			
9	25.317	1551	2(5H)-Furanone, 4-methyl-5,5-bis(2-methyl-2-propenyl)-	$C_{13}H_{18}O_{2}$			
10	25.462	1556	Dodecanoic acid	C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>			
11	25.694	1564	2-Oxabicyclo[3.3.0]oct-7-en-3-one, 7-(1-hydroxypentyl)-	$C_{12}H_{18}O_3$			
12	25.922	1571	Dodecane, 2,6,10-trimethyl-	$C_{15}H_{32}$			
13	26.114	1577	Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester	C <sub>16</sub> H <sub>30</sub> O <sub>4</sub>			
14	26.335	1584	3-Butyl-4-nitro-pent-4-enoic acid, methyl ester	$C_{10}H_{17}NO_4$			
15	26.514	1590	2-Dodecen-1-yl(-)succinic anhydride	C <sub>16</sub> H <sub>26</sub> O <sub>3</sub>			
16	26.838	1600	Heptadecane	C <sub>17</sub> H <sub>36</sub>			
17	27.227	1611	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	C <sub>9</sub> H <sub>10</sub> O <sub>4</sub>			
18	27.929	1629	2,6,10,10-Tetramethyl-1-oxaspiro-[4.5]decan-6-ol	$C_{13}H_{24}O_{2}$			
19	28.288	1638	4-Isobenzofuranol, octahydro-3a,7a-dimethyl-, (3a.alpha.,4.beta.,7a.alpha.)-(.+)-	$C_{10}H_{18}O_{2}$			
20	29.187	1662	Ethanol, 2-(hexadecyloxy)-	$C_{18}H_{38}O_2$			
21	29.827	1679	2-Cyclohexen-1-one, 3-(3-hydroxybutyl)-2,4,4-trimethyl-	C <sub>13</sub> H <sub>22</sub> O <sub>2</sub>			
22	29.956	1682	Cyclopentanone, 2-(1-adamantyl)-	$C_{15}H_{22}O$			
23	30.308	1692	alpha. Isomethyl ionone	$C_{14}H_{22}O$			
24	30.649	1700	2-Bromotetradecane	C <sub>14</sub> H <sub>29</sub> Br			
25	31.047	1710	Hexadecane, 2,6,10,14-tetramethyl-	C <sub>20</sub> H <sub>42</sub>			
26	31.774	1727	Adamantane, 1-thiocyanatomethyl-	C <sub>12</sub> H <sub>17</sub> NS			
27	32.083	1734	E,E-6,8-Tridecadien-2-ol, acetate	$C_{15}H_{26}O_{2}$			
28	32.522	1744	1-Decanol, 2-hexyl-	$C_{16}H_{34}O$			
29	32.801	1751	7-Methyl-Z-tetradecen-1-ol acetate	C <sub>17</sub> H <sub>32</sub> O <sub>2</sub>			
30	33.682	1771	7-Bromo-3a,6,6-trimethyl-hexahydro-benzofuran-2(3H)-one	$C_{11}H_{17}BrO_2$			
31	35.475	1813	Heptadecane, 2,6,10,15-tetramethyl-	C <sub>21</sub> H <sub>44</sub>			
32	35.876	1822	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	$C_{16}H_{22}O_4$			
33	37.903	1867	Dodecane, 1,2-dibromo-	$C_{12}H_{24}Br_2$			
34	39.916	1912	Dibutyl phthalate	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>			
35	41.653	1951	n-Hexadecanoic acid	$C_{16}H_{32}O_{2}$			
36	65.178	2500	1,2-Benzenedicarboxylic acid, diisooctyl ester	$C_{24}H_{38}O_4$			
37	73.760	2726	13-Docosenamide, (Z)-	C <sub>22</sub> H <sub>43</sub> NO			
38	93.411	3301	1,2-Benzenedicarboxylic acid, diundecyl ester	C <sub>30</sub> H <sub>50</sub> O <sub>4</sub>			
39	93.650	3307	Isophthalic acid, allyl pentadecyl ester	$C_{26}H_{40}O_4$			
40	100.522	3505	9-Octadecenoic acid (Z)-, phenylmethyl ester	$C_{25}H_{40}O_{2}$			
41	101.150	3525	2,6-Lutidine 3,5-dichloro-4-dodecylthio-	$C_{19}H_{31}Cl_2NS$			
42	102.301	3562	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester C <sub>35</sub> F				

Table 3: List of the hydrophilic volatile component identified from the stem skin of the Ilex cornuta Lindl. & Paxton.

Note: The bold and italic fonts are used to refer to exclusive compounds. RT: Retention time. RI: Reflex index.

No	RT	RI	Compound	Molecular
1	13.543	1196	2-Furancarboxaldehyde, 5-(hydroxymethyl)-	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>
2	14.110	1212	2-Furancarboxaldehyde, 6-(hydroxymethyl)-	$C_6H_6O_4$
3	14.318	1218	2-Furancarboxaldehyde, 7-(hydroxymethyl)-	$C_6H_6O_5$
4	25.089	1544	Bicyclo[3.2.0]heptan-6-one, 2-acetyl-3,3-dimethyl-7-(1-methylethyl)-	$C_{14}H_{22}O_{2}$
5	25.453	1556	Dodecanoic acid	$C_{12}H_{24}O_{2}$
6	25.692	1564	trans-ZalphaBisabolene epoxide	C <sub>15</sub> H <sub>24</sub> O
7	26.117	1577	4,6,10,10-Tetramethyl-5-oxatricyclo[4.4.0.0(1,4)]dec-2-en-7-ol	$C_{13}H_{20}O_{2}$
8	26.493	1589	7-Heptadecene, 1-chloro-	$C_{17}H_{33}Cl$
9	26.831	1600	Hexadecane	C <sub>16</sub> H <sub>34</sub>
10	28.088	1633	3-Pyridinecarboxylic acid, 1,6-dihydro-4-hydroxy-2-methyl-6-oxo-, ethyl ester	C <sub>9</sub> H <sub>11</sub> NO <sub>4</sub>
11	30.644	1700	Heptadecane	C <sub>17</sub> H <sub>36</sub>
12	31.038	1710	Hexadecane, 2,6,11,15-tetramethyl-	$C_{20}H_{42}$
13	32.440	1742	2-Cyclohexen-1-one, 4-hydroxy-3,5,6-trimethyl-4-(3-oxo-1-butenyl)-	$C_{13}H_{18}O_{3}$
14	32.801	1751	7-Methyl-Z-tetradecen-1-ol acetate	C <sub>17</sub> H <sub>32</sub> O <sub>2</sub>
15	34.479	1790	Pentadecyl trifluoroacetate	C <sub>17</sub> H <sub>31</sub> F <sub>3</sub> O <sub>2</sub>
16	34.925	1800	Heptadecane, 2,6,10,15-tetramethyl-	C <sub>21</sub> H <sub>44</sub>
17	35.476	1813	Nonadecane	C <sub>19</sub> H <sub>40</sub>
18	35.872	1822	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>
19	41.601	1949	n-Hexadecanoic acid	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>
20	43.458	1991	1-Nonadecene	C <sub>19</sub> H <sub>38</sub>
21	59.608	2362	2-Methyloctadecan-7,8-diol	C <sub>19</sub> H <sub>40</sub> O <sub>2</sub>
22	73.760	2726	13-Docosenamide, (Z)-	C <sub>22</sub> H <sub>43</sub> NO
23	92.239	3268	Isophthalic acid, allyl pentadecyl ester	C <sub>26</sub> H <sub>40</sub> O <sub>4</sub>
24	93.235	3296	1,2-Benzenedicarboxylic acid, 2-butoxyethyl butyl ester	$C_{18}H_{26}O_5$
25	94.006	3317	Phthalic acid, propyl octadecyl ester	$C_{29}H_{48}O_4$

#### Table 4: List of the hydrophilic volatile component of the leaf of the Ilex cornuta Lindl. & Paxton.

 Table 5: List of the hydrophilic volatile component identified from the flower of the Ilex cornuta Lindl. & Paxton.

No	RT	RI	Compound	Molecular
1	9.359	1070	2,2-Dimethyl-3-vinyl-bicyclo[2.2.1]heptane	$C_{_{11}}H_{_{18}}$
2	9.987	1091	Cyclohex-3-enecarboxaldehyde, 2,4,6-trimethyl-, oxime	$C_{10}H_{17}NO$
3	12.197	1156	Phenol, 3-ethyl-	$C_{8}H_{10}O$
4	12.649	1170	Benzoic acid	$C_7H_6O_2$
5	12.797	1174	Glucosamine, N-acetyl-N-benzoyl-	$C_{15}H_{19}NO_7$
6	13.333	1190	Benzothiazole	$C_7 H_5 NS$
7	15.613	1256	Phenol, 2,3,5-trimethyl-	$C_{g}H_{12}O$
8	16.214	1273	5H-Inden-5-one, 1,2,3,6,7,7a-hexahydro-	$C_{g}H_{12}O$
9	16.640	1286	Hydroquinone	$C_6 H_6 O_2$
10	17.145	1300	Cyclohexanol, 1-methyl-4-(1-methylethylidene)-	$C_{_{10}}H_{_{18}}O$
11	17.280	1304	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, (1.alpha.,2.beta.,5.alpha.)-	$C_{_{10}}H_{_{18}}O$
12	17.772	1319	2,7-Octadiene-1,6-diol, 2,6-dimethyl-	$C_{10}H_{18}O_{2}$
13	18.160	1330	trans-ZalphaBisabolene epoxide	C <sub>15</sub> H <sub>24</sub> O
14	18.430	1338	(3S,4R,5R,6R)-4,5-Bis(hydroxymethyl)-3,6-dimethylcyclohexene	$C_{10}H_{18}O_{2}$
15	19.298	1364	4-Hydroxy-2-methoxybenaldehyde	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>
16	19.508	1370	2-Cyclopenten-1-one, 4-hydroxy-3-methyl-2-(2-propenyl)-	$C_9H_{12}O_2$
17	21.040	1417	Phenol, 2-pentyl-	$C_{_{11}}H_{_{16}}O$
18	21.311	1425	2-Propen-1-ol, 2-methyl-3-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (E)-	$C_{13}H_{22}O$
19	21.602	1434	3-(2-Hydroxy-cyclopentylidene)-2-methyl-propionic acid	$C_{g}H_{14}O_{3}$

20	21.838	1442	5-Benzofuranacetic acid, 6-ethenyl-2,4,5,6,7,7a-hexahydro-3,6-dimethyl-α-methylene-2-oxo-, methyl ester	$C_{16}H_{20}O_4$
21	23.259	1486	8-Methylenecyclooctene-3,4-diol	$C_{g}H_{14}O_{2}$
22	23.514	1494	1-(3,6,6-Trimethyl-1,6,7,7a-tetrahydrocyclopenta[c]pyran-1-yl)ethanone	$C_{13}H_{18}O_{2}$
23	24.011	1509	1-Acetamido-1,2-dihydro-2-oxopyridine	$C_{7}H_{8}N_{2}O_{2}$
24	24.675	1531	cis-ZalphaBisabolene epoxide	$C_{15}H_{24}O$
25	24.767	1534	Cyclopentan-1-al, 4-isopropylidene-2-methyl-	$C_{10}H_{16}O$
26	25.085	1544	Ethanone, 1-(1a,2,3,5,6a,6b-hexahydro-3,3,6a-trimethyloxireno[g]benzofuran-5-yl)-	$C_{13}H_{18}O_{3}$
27	25.514	1558	Dodecanoic acid	C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>
28	25.685	1563	Bicyclo[3.3.1]nonan-9-one, 1,2,4-trimethyl-3-nitro-, (2-endo,3-exo,4-exo)-(.+)-	$C_{12}H_{19}NO_3$
29	25.899	1570	2-Cyclohexen-1-one, 3-(3-hydroxybutyl)-2,4,4-trimethyl-	C <sub>13</sub> H <sub>22</sub> O <sub>2</sub>
30	26.127	1578	Ledol	$C_{15}H_{26}O$
31	26.498	1590	1-Hexadecanol	C <sub>16</sub> H <sub>34</sub> O
32	26.840	1600	Hexadecane	C <sub>16</sub> H <sub>34</sub>
33	27.155	1609	Spiro[androst-5-ene-17,1'-cyclobutan]-2'-one, 3-hydroxy-, (3.beta.,17.beta.)-	$C_{22}H_{32}O_{2}$
34	27.486	1617	Bicyclo[3.1.0]hexane-6-methanol, 2-hydroxy-1,4,4-trimethyl-	$C_{10}H_{18}O_2$
35	28.099	1634	3-Pyridinecarboxylic acid, 1,6-dihydro-4-hydroxy-2-methyl-6-oxo-, ethyl ester	C <sub>9</sub> H <sub>11</sub> NO <sub>4</sub>
36	28.615	1647	Bromoacetic acid, dodecyl ester	$C_{14}H_{27}BrO_2$
37	28.684	1649	Chloroacetic acid, 4-tetradecyl ester	$C_{16}H_{31}ClO_2$
38	29.178	1662	2-Dodecen-1-yl(-)succinic anhydride	C <sub>16</sub> H <sub>26</sub> O <sub>3</sub>
39	29.777	1678	2-Hydroxy-1,1,10-trimethyl-6,9-epidioxydecalin	$C_{13}H_{22}O_{3}$
40	29.951	1682	1-Cyclopropene-1-pentanol, .alpha.,.epsilon.,.epsilon.,2-tetramethyl-3-(1-methylethenyl)-	$C_{15}H_{26}O$
41	30.651	1701	2-Bromotetradecane	C <sub>14</sub> H <sub>29</sub> Br
42	31.045	1710	Tetradecane, 1-chloro-	$C_{_{14}}H_{_{29}}Cl$
43	31.355	1717	5. beta.,7. beta.H,10. alphaEudesm-11-en-1. alphaol	$C_{15}H_{26}O$
44	31.582	1722	7-Hexadecenal, (Z)-	C <sub>16</sub> H <sub>30</sub> O
45	31.771	1727	Pentane-2,4-dione, 3-(1-adamantyl)-	$C_{15}H_{22}O_{2}$
46	32.092	1734	Butanol, 1-[2,2,3,3-tetramethyl-1-(3-methyl-1-penynyl)-cyclopropyl]-	C <sub>17</sub> H <sub>30</sub> O
47	32.468	1743	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-	$C_{11}H_{18}N_2O_2$
48	32.769	1750	Tetradecanoic acid	$C_{14}H_{28}O_{2}$
49	33.645	1771	1-Decanol, 2-hexyl-	C <sub>16</sub> H <sub>34</sub> O
50	34.485	1790	Pentadecyl trifluoroacetate	$C_{17}H_{31}F_{3}O_{2}$
51	34.932	1801	Heptadecane, 2,6,10,15-tetramethyl-	$C_{21}H_{44}$
52	35.479	1813	1-Octanol, 2-butyl-	$C_{12}H_{26}O$
53	35.873	1822	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	$C_{16}H_{22}O_4$
54	36.928	1845	5,10-Diethoxy-2,3,7,8-tetrahydro-1H,6H-dipyrrolo[1,2-a;1',2'-d]pyrazine	$C_{14}H_{22}N_2O_2$
55	37.910	1867	2-Hexadecene, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-	$C_{20}H_{40}$
56	39.389	1900	Nonadecane	C <sub>19</sub> H <sub>40</sub>
57	41.675	1951	n-Hexadecanoic acid	$C_{16}H_{32}O_{2}$
58	43.480	1991	1-Nonadecene	C <sub>19</sub> H <sub>38</sub>
59	46.996	2069	3-Chloropropionic acid, heptadecyl ester	C <sub>20</sub> H <sub>39</sub> ClO <sub>2</sub>
60	48.984	2114	9,12-Octadecadienoic acid (Z,Z)-	C <sub>18</sub> H <sub>32</sub> O <sub>2</sub>
61	49.228	2120	9-Octadecenal, (Z)-	C <sub>18</sub> H <sub>34</sub> O
62	50.660	2152	Ethyl iso-allocholate	C <sub>26</sub> H <sub>44</sub> O <sub>5</sub>
63	52.394	2192	9-Tricosene, (Z)-	C <sub>23</sub> H <sub>46</sub>
64	73.770	2727	13-Docosenamide, (Z)-	C <sub>22</sub> H <sub>43</sub> NO

Note: The bold and italic fonts are used to refer to exclusive compounds. RT: Retention time. RI: Reflex index.

No	RT	RI	Compound	Molecular			
1	9.133	1063	Mequinol	$C_7 H_8 O_2$			
2	9.303	1069	Phenol, 4-methyl-	$C_{T}H_{8}O$			
3	9.430	1073	Hexane, 3-bromo-	$C_6H_{13}Br$			
4	9.923	1089	Phenylethyl Alcohol	$C_8H_{10}O$			
5	10.510	1107	4-Acetylbutyric acid	$C_{6}H_{10}O_{3}$			
6	12.643	1169	Benzoic acid	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>			
7	13.559	1196	2-Furancarboxaldehyde, 5-(hydroxymethyl)-	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>			
8	15.378	1249	1,5-Cyclooctadien-4-one	$C_8H_{10}O$			
9	17.652	1315	Phenol, 2,6-dimethoxy-	$C_{8}H_{10}O_{3}$			
10	19.180	1361	Benzaldehyde, 3-hydroxy-4-methoxy-	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>			
11	21.852	1442	2-Ethoxyphenylacetonitrile	$C_{10}H_{11}NO$			
12	22.103	1450	Benzeneacetonitrile, 4-hydroxy-	C <sub>8</sub> H <sub>7</sub> NO			
13	22.466	1461	Coumarin, 8-methyl-	$C_{10}H_8O_2$			
14	25.187	1547	1,4-Benzenediol, 2-(1,1-dimethylethyl)-	$C_{10}H_{14}O_{2}$			
15	25.508	1558	Dodecanoic acid	C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>			
16	25.876	1569	3,5-Octadienoic acid, 7-hydroxy-2-methyl-, [R*,R*-(E,E)]-	$C_{q}H_{14}O_{3}$			
17	25.938	1571	2-Cyclopenten-1-one, 4-hydroxy-3-methyl-2-(2-propenyl)-	C <sub>9</sub> H <sub>12</sub> O <sub>2</sub>			
18	26.125	1577	1b,5,5,6a-Tetramethyl-octahydro-1-oxa-cyclopropa[a]inden-6-one	$C_{13}H_{20}O_{2}$			
19	26.492	1589	4-Chloro-3-n-hexyltetrahydropyran	$C_{11}H_{21}ClO$			
20	27.323	1613	Ethanone, 1-[2-(5-hydroxy-1,1-dimethylhexyl)-3-methyl-2-cyclopropen-1-yl]-	C <sub>14</sub> H <sub>24</sub> O <sub>2</sub>			
21	30.643	1700	Heptadecane	C <sub>17</sub> H <sub>36</sub>			
22	32.760	1750	Tetradecanoic acid	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>			
23	35.878	1822	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>			
24	41.694	1952	n-Hexadecanoic acid	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>			
25	48.863	2111	9,12-Octadecadienoic acid, methyl ester	$C_{19}H_{34}O_{2}$			
26	49.244	2120	9-Octadecenal, (Z)-	C <sub>18</sub> H <sub>34</sub> O			

Table 6: List of the hydrophilic volatile component identified from the fruit of the Ilex cornuta Lindl. & Paxton.

Note: The bold and italic fonts are used to refer to exclusive compounds. RT: Retention time. RI: Reflex index.

Table 7: The number and percentage of the common and exclusive hydrophilic volatile compounds identified from the six organs.

Organ	Root	Stem	Stem Skin	Leaf	Flower	Fruit
Total Compounds	36	46	42	25	64	26
Common Compounds	3					
Percentage of Common Compounds	8.3%	6.5%	7.1%	12.0%	4.7%	11.5%
Exclusive Compounds	17	21	21	9	40	15
Percentage of Exclusive Compounds	47.2%	45.7%	50.0%	36.0%	62.5%	57.7%

practice of the traditional herbal medicine to treat the diseases using either the whole plant or part of the plants depending on which part contains the substances that can be used for therapeutic purposes.

Table 8 presents the number of overlapping compounds, overlapping percentage and overlapping index. The stem and stem skin share the largest number (15) of overlapping compounds. The overlapping percentage is calculated to be 32.6% for the stem and 35.7% for the stem skin. The smallest number (5) of overlapping compounds are found between root and fruit, leaf and fruit. The percentage of overlapping compounds between each of the two organs ranges from 10.9% to 44.0%, which is relatively small, further demonstrating substantial component differences among the different organs. The overlapping index is used to reveal the similarity among the organs. Two organs share the same number of overlapping compounds, but the overlapping index could be different if the total number of the hydrophilic volatile compounds, the less the percentage of the overlapping compounds and smaller the overlapping index.

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That is why the average overlapping indices between the two organs is introduced to normalize the difference. In addition, total average overlapping indices is derived to calculate the mean of the average overlapping indices between each organ and the other five organs. Based on Table 8, the total average overlapping indices for each organ follows the order of stem > stem skin > root > leaf > flower > fruit. The total average overlapping indices for the stem is the greatest at 3.056, indicating the stem share the maximum similarity with the plant. The total average overlapping indices for the fruit was the smallest at 1.090, indicating that the fruit share the minimum similarity with the plant. And there is not much difference in the average overlapping indices between fruit and the other five organs. Except fruit, the average overlapping indices between each of the two organs correlate well to their physical proximity. The root, stem and stem skin are the organs that the plant survive and grow, and their total average overlapping indices are greater than 2.5. The overlapping index differences among these three organs are small, and they share the most in common. As an evergreen plant, the leaf is symbiotically related to the plant

Organ 1	Organ 2	Number of overlapping compounds	Overlapping percentage	Overlapping index for Organ 1	Overlapping index for Organ 2	Average overlapping indices between organ 1 and 2	Total average overlapping Indices
	Stem	14	38.9%	5.444	4.261	4.853	
	Stem skin	11	30.6%	3.361	2.881	3.121	
Root	Leaf	9	25.0%	2.250	3.240	2.745	
	Flower	7	19.4%	1.361	0.766	1.064	2.522
	Fruit	5	13.9%	0.694	0.962	0.828	
	Root	14	30.4%	4.261	5.444	4.853	
	Stem skin	15	32.6%	4.891	5.357	5.124	
Stem	Leaf	9	19.6%	1.761	3.240	2.501	
	Flower	10	21.7%	2.174	1.266	1.720	3.056
	Fruit	6	13.0%	0.783	1.385	1.084	
	Root	11	26.2%	2.881	3.361	3.121	
	Stem	15	35.7%	5.357	4.891	5.124	
Stem skin	Leaf	9	21.4%	1.929	3.240	2.585	
	Flower	10	21.4%	1.929	1.266	1.598	2.710
	Fruit	6	14.3%	0.857	1.385	1.121	
	Root	9	36.0%	3.240	2.250	2.745	
	Stem	9	36.0%	3.240	1.761	2.501	
Leaf	Stem skin	9	36.0%	3.240	1.929	2.585	
	Flower	11	44.0%	4.840	1.891	3.366	2.435
	Fruit	5	20.0%	1.000	0.962	0.981	
	Root	7	10.9%	0.766	1.361	1.064	
	Stem	10	15.6%	1.563	2.174	1.859	
Flower	Stem skin	10	14.1%	1.266	1.929	1.598	
	Leaf	11	17.2%	1.891	4.840	3.366	1.844
	Fruit	7	10.9%	0.766	1.885	1.326	
	Root	5	19.2%	0.962	0.694	0.828	
	Stem	6	23.1%	1.385	1.000	1.193	
Fruit	Stem skin	6	23.1%	1.385	0.857	1.121	
	Leaf	5	19.2%	0.962	1.000	0.981	1.090
	Flower	7	26.9%	1.885	0.766	1.326	

Table 8: The number of overlapping compounds, overlapping percentage and overlapping index.

although the relationship between each leaf and the plant is cyclical, so the leaf is secondarily related to the plant. The flower and fruit are also cyclically related to the plant and have the most distant relationship. The leaf, flower and fruit are necessary but not survival organs for the growth of the plant. The relationship between the organs and the plant generated from the analysis of the hydrophilic volatile compounds is consistent with their biological function.

## Conclusion

The root, stem, stem skin, leaf, flower and fruit of the *llex cornuta* Lindl. & Paxton contain hydrophilic volatile compounds that are evenly distributed in the water phase of the various organs of the plant and can volatilize with water vapor. The number and type of hydrophilic volatile compounds vary from organ to organ. There is only a small number of common compounds among the six organs and the number of overlapping compounds between each of the two

organs is also relatively small. In addition, there are large number of exclusive compounds from each organ. Therefore, it is possible to identify the plant through the assessment of the hydrophilic volatile compounds isolated from each individual organ.

In conclusion, we found that hydrophilic volatile metabolites are a class of natural products that are rarely investigated but constitute a significant part of the plant chemical composition. Chemical profiling of these secondary metabolites could provide a valuable tool for identification and authentication of the plant samples, as well as resolving taxonomic problems and understanding the chemically mediated biological phenomena.

### References

 Bickford D, Lohman DJ, Sodhi NS, Ng PKL, Meier R, et al. (2007) Cryptic species as a window on diversity and conservation. *Trends Ecol Evol* 22: 148-155. [crossref]

- Heinrichs J, Kreier HP, Feldberg K, Schmidt AR, Zhu RL, et al. (2011) Formalizing morphologically cryptic biological entities: New insights from DNA taxonomy, hybridization, and biogeography in the leafy liverwort Porella platyphylla (Jungermanniopsida, Porellales). *Am J Bot* 98: 1252-1262. [crossref]
- 3. Ludwiczuk A (2014) Fingerprinting of secondary metabolites of liverworts: chemosystematic approach. *J of AOAC Int* 97: 1234-1243.
- 4. Wink M (2003) Evolution of secondary metabolites from an ecological and molecular phylogenetic perspective. *Phytochemistry* 64: 3-19. [crossref]
- Liu K, Abdullah AA, Huang M, Nishioka T, Altaf-Ul-Amin M, et al. (2017) Novel Approach to Classify Plants Based on Metabolite-Content Similarity. *BioMed Res Int.* doi: 10.1155/2017/5296729
- Ghaste M, Narduzzi L, Carlin S, Vrhovsek U, Shulaev V, et al. (2015) Chemical Composition of Volatile Aroma Metabolites and Their Glycosylated Precursors that Can Uniquely Differentiate Individual Grape Cultivars. *Food Chem* 188: 309-319. [crossref]
- Peters K, Treutler H, Doll S, Kindt ASD, Hankemeier T, et al. (2019) Chemical Diversity and Classification of Secondary Metabolites in Nine Bryophyte Species. *Metabolites* 9: 222. [crossref]
- Staszek D, Orlowska M, Rzepa J, Wrobel MS, Kowalska T (2014) Fingerprinting of the Volatile Fraction from Selected Thyme Species by Means of Headspace Gas Chromatography with Mass Spectrometric Detection. J of AOAC Int 97: 1250-1258. [crossref]

- Tundis R, Peruzzi L, Menichini F (2014) Phytochemical and biological studies of Stachy Species in Relation to Chemotaxonomy: A Review. *Phytochemistry* 102: 7-39. [crossref]
- Peñuelas J, Llusià J (1999) Seasonal emission of monoterpenes by the Mediterranean tree Quercus ilex in field conditions: Relations with photosynthetic rates, temperature and volatility. *Physiol Plant* 105: 641-647.
- Llusia J, Penuelas J (2000) Seasonal patterns of terpene content and emission from seven mediterranean woody species in field conditions. *Am J Bot* 87: 133-140. [crossref]
- Ormeo E, Goldstein A, Niinemets ü (2011) Extracting and trapping biogenic volatile organic compounds stored in plant species. TRAC-Trend Anal Chem 30: 978-989.
- Claudia G, Roberta A, Daniela L, Giacomo T, Laura S, et al. (2018) Salvia verticillata: Linking glandular trichomes, volatiles and pollinators. *Phytochemistry* 155: 53-60.
- Wei X, Song M, Chen C, Tong H, Liang G, et al. (2018) Juice volatile composition differences between Valencia orange and its mutant Rohde Red Valencia are associated with carotenoid profile differences. *Food Chem* 245: 223-232. [crossref]
- Berlinck RGS, Monteiro AF, Bertonha AF, Bernardi DI, Gubiani JR, et al. (2019) Approaches for the isolation and identification of hydrophilic, light-sensitive, volatile and minor natural products. *Nat Prod Rep* 36: 981-1004. [crossref]

#### Citation:

Huang L (2021) Chemical Composition Similarity Relationships among the Various Organs of the *Ilex Cornuta* Lindl. & Paxton Based on the Analysis of Hydrophilic Volatile Compounds. *Internal Med Res Open J* Volume 6(2): 1-10.