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Volatile Organic Compounds of Marine Sponge Petrosia ficiformis from the Adriatic Sea

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Abstract: Volatile organic compounds (VOCs) of Petrosia ficiformis were investigated for the first time. The VOCs from fresh and air-dried sponge were obtained by hydrodistillation and headspace-solid phase microextraction and they were analysed by coupled gas chromatography-mass spectrometry. Aliphatic compounds with octan-3-one (up to 24.02 %), oct-1-en-3-ol (up to 8.65 %) and heptadecane (up to 39.37 %) were the most abundant in the fresh sponge along with benzaldehyde (up to 18.59 %) and diisobutyl phthalate (up to 8.44 %). Higher percentage of N,N-dimethylmethanamine (up to 19.08 %) was found in dried sample headspace and the loss of octan-3-one and benzaldehyde and increase of benzyl alcohol (up to 18.90%) were noted. The great difference among the fresh and dried sponge VOCs obtained by hydrodistillation was noticed for fatty acids and derivatives abundance and 1H-indole increased (up to 6.00 %) in the dried sponge. Both methods enabled obtaining more complete VOCs profile and drying significantly changed their composition.

Keywords: Petrosia ficiformis (Poiret, 1789), GC-MS, hydrodistillation, headspace, heptadecane, oct-1-en-3-ol, octan-3-one, benzyl alcohol, benzaldehyde, diisobutyl phthalate, N,N-dimethylmethanamine, dimethyl trisulphide, 1H-indole.

INTRODUCTION

Detrosia is one of 4 genera of Petrosiidae family belonging to the order Haplosclerida, which is known among sponges as the most prolific source of secondary metabolites.^[1] Petrosia genus includes 122 species belonging to two subgenera (Petrosia and Strongylophora) according to the Word Register of Marine Species (WoRMS). A recent review paper compared secondary metabolites isolated from the sponges of the genus Petrosia.^[2] It was reported that associated microorganisms can account for up to 60 % of the fresh weight of marine sponges and it is believed that these sponge-associated microorganisms (such as bacteria, fungi, cyanobacteria, and unicellular algae) may be involved in the biosynthesis of natural products.^[3]

Petrosia ficiformis (Poiret, 1789; Haplosclerida, Petrosiidae) is a marine sponge found across the Mediterranean and in the Eastern Atlantic.^[4] The mixtures of high-molecular weight polyacetylenes with 46-55 carbons were isolated from P. ficiformis.^[5] Five additional polyacetylenes up to 52 carbons, isolated from P. ficiformis from the Mediterranean Sea, were also reported.^[6] Polyacetylenes with two terminal 1-yn-3-ol-4-ene moieties and 46 total carbons isolated from Mediterranean P. ficiformis were identified and evaluated for their biological activity. It was found that they inhibit sea urchin egg development and act as a potent toxin against Artemia salina.^[7,8] Petroformynes, isopetroformynes, and various oxidized or isomerized analogues were reported in P. ficiformis and most of these analogues exhibited lethality against brine shrimp.^[7–10] Sterols have rarely been isolated from Petrosia sponges in temperate regions, but P. ficiformis contains sterol compounds with cyclopropane in the branch at C-17.^[2] Petrosterol (26,27-cycloaplysterol), a steroid with a cyclopropane ring at C-25 and C-26, was isolated from P. ficiformis collected in the Bay of Naples and later ficisterol (23-ethyl-24-methyl-27-norcholesta-5,25dien-3 β -ol) was found as the minor component.^[11–13] The relative abundance of phospholipids classes varies with sponge species, but amino phospholipids, especially phosphatidylethanolamine and phosphatidylcholine were found in P. ficiformis.^[14] Its phospholipids also included numerous branched fatty acids (e.g. (Z,Z)-25-methylhexa-



cosa-5,9-dienoic acid and (*Z*,*Z*)-24-methylhexacosa-5,9-dienoic acid).^[14]

There were no data about volatile organic compounds (VOCs) of this marine sponge that are the focus of this investigation. The present research has the following key goals: a) isolate VOCs of fresh *P. ficiformis* (FrPF) and air-dried *P. ficicormis* (DrPF) retrieved by both headspace solid-phase microextraction (HS-SPME) and hydrodistillation (HD); b) identify the isolated VOCs by gas chromatography–mass spectrometry analysis (GC-MS); b) compare VOCs of FrPF and DrPF.

EXPERIMENTAL

Marine Sponge Sample

P. ficiformis sample was collected in the Adriatic Sea near Rtina peninsula (Island of Pag), with the exact geographical location being: 44° 19' 10" N; 15° 15' 37" E. The sampling depth was 6 m with a sea temperature of 18 °C. Upon collection, the sample was placed in an airtight container filled with seawater and immediately delivered to the laboratory. Until processing, the fresh sample was stored and kept in the laboratory freezer, while the air-dried sample was kept in the dark at room temperature for 10 days. Before the analysis, the used sponge sample was cleaned of stones and other visible foreign matters. Both fresh and air-dried sponge samples were sliced into small pieces and used for headspace solid-phase microextraction (HS-SPME) and hydrodistillation (HD).

Headspace Solid-Phase Microextraction (HS-SPME)

HS-SPME was performed with PAL Auto Sampler System (PAL, RSI 85, CTC Analytics AG, Switzerland) using SPME fibres with PDMS/DVB (polydimethylsiloxane/divinylbenzene) and DVB/CAR/PDMS (divinylbenzene/carboxene/ polydimethylsiloxane) coatings. Both fibres were obtained from Agilent Technologies (Santa Clara, CA, USA). Prior to the use, the fibres were conditioned according to the manufacturer's instructions. 1 g of fresh or dry sponge sample was placed into 20 mL glass vials and hermetically sealed with a screw cap containing polytetrafluoroethylene (PTFE)/silicone septum. The samples were equilibrated for 15 min at 60 °C and then extracted for 45 min. The injector temperature was set to 250 °C and thermal desorption was carried out for 6 min directly to the GC column. HS-SPME was performed in triplicate.

Hydrodistillation (HD)

Modified Clevenger apparatus with pentane (Kemika, Zagreb, Croatia) and diethyl ether (Kemika, Zagreb, Croatia) solvent trap (v/v ratio 1:2) was used for distillation. 100 g of

fresh sample and 30 g of air-dried sample were used separately. HD was carried out for 2 hours. After HD, the solvent trap layer was carefully separated using a glass pipette, concentrated by the slow flow of nitrogen up to 0.05 mL and later used for GC-MS analysis.

Gas Chromatography-Mass Spectrometry (GC-MS) Analysis of VOCs

GC-MS analysis was carried out on Agilent Technologies (Palo Alto, CA, USA) gas chromatograph model 8890A equipped with mass selective detector model 5977E. Separation of the compounds was achieved on an HP-5MS column (Agilent Technologies, Santa Clara, CA, USA) 30 m x 0.25 mm containing a non-polar stationary phase (5 % diphenyl / 95 % dimethylpolysiloxane) and 0.25 μ m film thickness. The following operating conditions for the gas chromatograph were used: 250 °C injector temperature; 300 °C detector temperature; column temperature program: 2 min isothermally at 70 °C, then temperature gradient from 70 °C to 200 °C at 3 °C/min and further retention for 15 min.

RESULTS AND DISCUSSIONS

Headspace Composition of VOCs isolated by HS-SPME

Headspace composition of both FrPF (HS-FrPF) and DrPF (HS-DrPF) were analysed using solid-phase microextraction (HS-SPME). Two fibres of different polarities were used: divinylbenzene/carboxene/polydimethylsiloxane (DVB/CAR/PDMS, f1) and polydimethylsiloxane/divinylbenzene (PDMS/DVB, f2) to get more profound headspace profile. In HS-FrPF 88.36 % (f1) and 89.22 % (f2) and in Hs-DrPF 95.46 % (f1) and 94.65 % (f2) of total VOCs were identified (Table 1).

Aliphatic compounds were dominant in both HS-FrPF (56.24 %, f1; 66.00 %, f2) and HS-DrPF (65.16 %, f1; 37.38 %, f2) (Figure 1) samples analysed with both fibres with octan-3-one (HS-FrPF, f1) and heptadecane (HS-FrPF, f2; HS-DrPF, both fibres) as two most abundant compounds (Figure 2). Octan-3-one, fatty acid derivative known as C₈-oxylipin,^[15] was identified only in HS-FrPF (24.02 %, f1; 15.39 %, f2). This compound was not detected after airdrying probably because of its high volatility. Several more C8-oxylipins were identified, such as oct-1-en-3-ol, oct-4en-3-ol, octan-2,3-dione, octan-2-one, octanal, (E)-oct-2en-1-al and volatile pheromone (3E,5Z)-octa-1,3,5-triene (fucoserratene) (Table 1). Heptadecane was the most abundant hydrocarbon. It is known that hydrocarbons are characteristic compounds for marine invertebrates and algae and form part of their defence system.^[16] It can be observed that the air-dried sponge sample analysed with f1 contains the largest share of this compound, 2.65 times higher than the analysed fresh sample on the same fibre **Table 1.** The volatile organic compounds isolated by headspace solid-phase microextraction (HS-SPME) and analysed by gas chromatography–mass spectrometry (GC-MS) from *P. ficiformis* samples: (I-fresh *P. ficiformis* extracted by DVB/CAR/PDMS fibre, II-air-dried *P. ficiformis* extracted by DVB/CAR/PDMS fibre, III-fresh *P. ficiformis* extracted by PDMS/DVB fibre, IV-air-dried *P. ficiformis* extracted by PDMS/DVB fibre).

ND. Component (soprophamine) AT I III IV 1 2. Aminopropane (isoprophamine) 470 1.5610.00 - - - - 2 N/A-Dimethylmethanamine 482 1.666.021 - 1.22.077 - - 2.380.10 3 Propan-2-01 510 - 1.22.077 - - 2.380.10 5 3-Methylbutan (isovaleraidehyde) 652 2.0340.38 - 1.1840.45 0.322.004 6 Pentanal 658 1.0410.20 - 0.4910.00 - 7 3-Methylbutan 1.01 (isoamyl alcohol) 734 - - - 0.5380.03 10 Pentanal 800 - 0.2410.07 - - - 3.8880.05 12 Hexanal 800 - 0.2410.07 - - - 0.660.00 - - 1.3880.05 - - 0.660.00 - - 0.660.00 - -	No	Commound	Ы	Area (%) ± SD*			
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16 Bromororm 892 - - 2.01±0.31 - 17 Heptanal 901 - 1.11±0.15 - 0.80±0.02 18 2,6-Dimethylpyrazine 922 - - - 0.82±0.05 19 2-Ethylhexan-1-al 954 - - 0.75±0.56 - 20 Benzaldehyde 961 18.59±1.87 2.68±0.02 10.82±4.56 5.33±0.29 21 3-Methylbutyl propanote (lsoamyl propionate) 969 - - 0.49±0.00 - 22 (Methyltrisulfanyl)methane (Dimethyl trisulfide) 972 - - 0.49±0.00 - 23 Oct-1-en-3-on 980 - - 0.40±0.07 - 24 Octan-2.3-dione 981 1.12±0.43 - 1.93±12.65 - 25 Octan-2.3-dione 987 - 0.75±0.22 - 0.78±0.12 26 Phenol 987 - 0.24±0.05 - 0.87±0.09 </td <td>15</td> <td>2.5-Diethvlfuran</td> <td>888</td> <td>_</td> <td>_</td> <td>_</td> <td>0.60±0.05</td>	15	2.5-Diethvlfuran	888	_	_	_	0.60±0.05
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18 2,6-Dimethylpyraine 922 - - - 0.8240.05 19 2-Ethylhexan-1-al 954 - - 0.75±0.56 - 20 Benzaldehyde 961 18.59±1.87 2.68±0.02 10.82±4.55 5.33±0.29 21 3-Methylbutyl propanota (Isoamyl propionate) 969 - - 0.66±0.04 22 (Methyltisulfanyl)methane (Dimethyl trisulfal) 970 - - 0.40±0.07 23 Oct-1-en-3-one 981 1.12±0.43 - - 0.40±0.07 24 Octan-2-one 984 24.02±0.38 - - 0.40±0.07 27 Octan-2,3-dione 984 24.02±0.33 - - 0.40±0.07 28 Octan-2,0 984 - - - 0.87±0.02 29 Octan-2,3-dione 984 - - - 0.87±0.02 29 Octan-2,0 992 - - 0.75±0.03 - 31	17	Heptanal	901	_	1.11±0.15	_	0.80±0.02
19 1.2. Hol Markin (Markin (Ma	18	2.6-Dimethylpyrazine	922	_	_	_	0.82+0.05
10 11<	19	2-Ethylbexan-1-al	954	_	_	0 75+0 56	_
21 3-Methylbutyl propanoate (isoamyl propionate) 969 - - 0.49±0.00 - 22 (Methyltrisulfanyl)methane (Dimethyl trisulfide) 972 - - 0.66±0.04 23 Oct-1-en-3-ol 980 - - 2.13±0.52 - 24 Oct-4-en-3-one 981 1.12±0.43 - - 0.40±0.07 25 Octan-2.3-dione 984 24.02±0.38 - 15.39±1.26 - 26 Phenol 984 24.02±0.38 - 0.78±0.12 - 27 Octan-2,3-dione 987 - - 0.78±0.12 - 28 Octan-2-one 992 - - 0.78±0.12 - 29 Octan-2,1ylbenzene (p-Cymene) 1026 - - 0.87±0.09 - 31 1.4,3,3-Trimethyl-2-oxabicycl0[2.2.2]octane (Eucalyptole) 1031 - - 1.50±1.22 - 33 2-Phenylmethanol (Benzyl alcohol) 1050 1.8±0.90 - 1.	20	Benzaldehvde	961	18.59+1.87	2.68+0.02	10.82+4.56	5.33+0.29
22 (Methyltrisulfanyl)methane (Dimethyl trisulfide) 972 - - - 0.66±0.04 23 Oct-1-en-3-ol 980 - - 2.13±0.52 - 24 Oct-4-en-3-one 981 1.12±0.43 - - 0.40±0.07 25 Octan-3-one 984 24.02±0.38 - 15.39±12.65 - 26 Phenol 984 - 0.77±0.22 - 1.98±0.12 27 Octan-2,3-dione 987 - - 0.78±0.10 - 28 Octan-2-one 992 - - 0.78±0.12 - 29 Octan-1/(propan-2-y)(benzene (p-Cymene) 1026 - - 0.87±0.09 30 1-Methyl-4-(propan-2-y)(benzene (p-Cymene) 1026 - - 1.07±0.49 - 31 1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane (Eucalyptole) 1031 - - 1.50±1.22 - 33 2-Phenylmethanol (Benzyl alcohol) 1063 0.49±0.18 - <td< td=""><td>21</td><td>3-Methylbutyl propanoate (Isoamyl propionate)</td><td>969</td><td>_</td><td>_</td><td>0.49+0.00</td><td>_</td></td<>	21	3-Methylbutyl propanoate (Isoamyl propionate)	969	_	_	0.49+0.00	_
123 (netrol, instance), instance), instance), instance,	22	(Methyltrisulfanyl)methane (Dimethyl trisulfide)	972	_	_	_	0.66+0.04
24 Oct-4-en-3-one 981 1.12±0.43 - - 0.40±0.07 25 Octan-3-one 984 24.02±0.38 - 15.39±12.65 - 26 Phenol 984 - 0.77±0.22 - 1.98±0.12 27 Octan-2,3-dione 987 - - 0.78±0.12 - 28 Octan-2,-one 992 - - 0.78±0.12 - 29 Octan-2-one 992 - - 0.78±0.12 - 30 1-Methyl-4-(propan-2-yl)benzene (p-Cymene) 1026 - - 0.24±0.05 - 31 1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane (Eucalyptole) 1031 - - 1.07±0.49 - 32 Phenylmethanol (Benzyl alcohol) 1042 1.61±0.15 14.78±1.62 - 18.90±0.46 33 2-Phenylacetaldehyde (Benzenacetaldehyde) 1050 1.8±0.90 - 1.50±1.22 - 34 (£)-Oct-2-enal 1063 0.49±0.15 -	23	Oct-1-en-3-ol	980	_	_	2 13+0 52	_
1 1	23	Oct-4-en-3-one	981	1 12+0 43	_	-	0 40+0 07
26 Phenol 984 - 0.77±0.22 - 1.98±0.12 27 Octan-2,3-dione 987 - - 0.78±0.12 - 28 Octan-2-one 992 - - 0.78±0.12 - 29 Octanal 1005 - - 0.87±0.09 30 1-Methyl-4-(propan-2-yl)benzene (p-Cymene) 1026 - - 0.24±0.05 - 31 1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane (Eucalyptole) 1031 - - 1.07±0.49 - 32 Phenylmethanol (Benzyl alcohol) 1042 1.61±0.15 14.78±1.62 - 18.90±0.46 33 2-Phenylacetaldehyde (Benzenacetaldehyde) 1050 1.8±0.90 - 1.50±1.22 - 34 (E)-Oct-2-enal 1063 0.49±0.18 - 0.75±0.28 - 35 1-Phenylethanone (Acetophenone) 1072 - - 0.55±0.08 - 36 Nonan-2-one 1091 0.66±0.06 - 0.34±0.00 - 37 Nonan-3-one 1091 - -	25	Octan-3-one	984	24 02+0 38	_	15 39+12 65	-
27 Octan-2,3-dione 987 - - - 0.78±0.12 28 Octan-2.one 992 - - 0.78±0.12 - 29 Octan-2.vljbenzene (p-Cymene) 1005 - - 0.87±0.09 30 1-Methyl-4-(propan-2-yljbenzene (p-Cymene) 1026 - - 0.24±0.05 - 31 1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane (Eucalyptole) 1031 - - 1.07±0.49 - 32 Phenylmethanol (Benzyl alcohol) 1042 1.61±0.15 14.78±1.62 - 18.90±0.46 33 2-Phenylacetaldehyde (Benzenacetaldehyde) 1050 1.8±0.90 - 1.50±1.22 - 34 (E)-Oct-2-enal 1063 0.49±0.18 - 0.76±0.22 - 35 1-Phenylethanone (Acetophenone) 1072 - - 0.55±0.08 - 36 Nonan-2-one 1091 0.66±0.06 - 0.34±0.00 - 37 Nonan-3-one 1091 - - 0.42±0.00 - 38 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one (Fe	25	Phenol	984	_	0 77+0 22	-	1 98+0 12
28 Octan 2,9 control 992 - - 0.78±0.12 - 29 Octan-2-one 992 - - 0.87±0.09 30 1-Methyl-4-(propan-2-yl)benzene (p-Cymene) 1026 - - 0.87±0.09 31 1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane (Eucalyptole) 1031 - - 1.07±0.49 - 32 Phenylmethanol (Benzyl alcohol) 1042 1.61±0.15 14.78±1.62 - 18.90±0.46 33 2-Phenylmethanol (Benzyl alcohol) 1042 1.61±0.15 14.78±1.62 - 18.90±0.46 34 (E)-Oct-2-enal 1063 0.49±0.18 - 0.76±0.22 - 35 1-Phenylethanone (Acetophenone) 1072 - - 0.55±0.08 - 36 Nonan-2-one 1091 0.66±0.06 - 0.34±0.00 - 37 Nonan-3-one 1091 - - 0.42±0.00 - 38 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one (Fenchone) 1096 -	20	Octan-2 3-dione	987	_	-	_	0.78+0.10
100 1000 - - - 0.87±0.09 30 1-Methyl-4-(propan-2-yl)benzene (p-Cymene) 1026 - - 0.87±0.09 31 1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane (Eucalyptole) 1031 - - 1.07±0.49 - 32 Phenylmethanol (Benzyl alcohol) 1042 1.61±0.15 14.78±1.62 - 18.90±0.46 33 2-Phenylmethanol (Benzyl alcohol) 1042 1.61±0.15 14.78±1.62 - 18.90±0.46 34 (E)-Oct-2-enal 1063 0.49±0.18 - 0.76±0.22 - 35 1-Phenylethanone (Acetophenone) 1072 - - 0.55±0.08 - 36 Nonan-2-one 1091 0.66±0.06 - 0.34±0.00 - 37 Nonan-3-one 1091 - - 0.42±0.00 - 38 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one (Fenchone) 1096 - - 0.34±0.00 - 39 3,7-Dimethylocta-1,6-dien-3-01 (Linalool) 1102	28	Octan-2-one	992	_	_	0 78+0 12	-
10 1026 - - 0.24±0.05 - 30 1-Methyl-4-(propan-2-yl)benzene (p-Cymene) 1026 - - 0.24±0.05 - 31 1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane (Eucalyptole) 1031 - - 1.07±0.49 - 32 Phenylmethanol (Benzyl alcohol) 1042 1.61±0.15 14.78±1.62 - 18.90±0.46 33 2-Phenylacetaldehyde (Benzenacetaldehyde) 1050 1.8±0.90 - 1.50±1.22 - 34 (E)-Oct-2-enal 1063 0.49±0.18 - 0.76±0.22 - 35 1-Phenylethanone (Acetophenone) 1072 - - 0.55±0.08 - 36 Nonan-2-one 1091 0.66±0.06 - 0.34±0.00 - 37 Nonan-3-one 1091 - - 0.42±0.00 - 38 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one (Fenchone) 1096 - - 0.34±0.00 - 39 3,7-Dimethylocta-1,6-dien-3-ol (Linalool) 110	20	Octanal	1005	_	_	-	0 87+0 09
31 1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane (Eucalyptole) 1031 - - 10.7±0.49 - 32 Phenylmethanol (Benzyl alcohol) 1042 1.61±0.15 14.78±1.62 - 18.90±0.46 33 2-Phenylacetaldehyde (Benzenacetaldehyde) 1050 1.8±0.90 - 1.50±1.22 - 34 (E)-Oct-2-enal 1063 0.49±0.18 - 0.76±0.22 - 35 1-Phenylethanone (Acetophenone) 1072 - - 0.55±0.08 - 36 Nonan-2-one 1091 0.66±0.06 - 0.34±0.00 - 37 Nonan-3-one 1091 - - 0.42±0.00 - 38 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one (Fenchone) 1096 - - 0.34±0.00 - 39 3,7-Dimethylocta-1,6-dien-3-ol (Linalool) 1102 - - 1.16±0.00 - 40 Nonanal 1102 - - - 2.41±0.13 41 2,6-Dimethylocyclohexan-1-ol 1110 - 0.97±0.21 - 1.78±0.15	30	1-Methyl-4-(propan-2-yl)benzene (n-Cymene)	1026	_	_	0 24+0 05	-
31 Phenylmethanol (Benzyl alcohol) 1031 14.78±1.62 - 18.90±0.46 32 Phenylmethanol (Benzyl alcohol) 1042 1.61±0.15 14.78±1.62 - 18.90±0.46 33 2-Phenylacetaldehyde (Benzenacetaldehyde) 1050 1.8±0.90 - 1.50±1.22 - 34 (E)-Oct-2-enal 1063 0.49±0.18 - 0.76±0.22 - 35 1-Phenylethanone (Acetophenone) 1072 - - 0.55±0.08 - 36 Nonan-2-one 1091 0.66±0.06 - 0.34±0.00 - 37 Nonan-3-one 1091 - - 0.42±0.00 - 38 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one (Fenchone) 1096 - - 0.34±0.00 - 39 3,7-Dimethylocta-1,6-dien-3-ol (Linalool) 1102 - - 1.16±0.00 - 40 Nonanal 1102 - - 1.78±0.15 1.78±0.15	31	1 3 3-Trimethyl-2-oxabicyclo[2 2 2]octane (Eucalyntole)	1031	_	_	1 07+0 49	_
31 2-Phenylacetaldehyde (Benzenacetaldehyde) 1051 10512015 1.051212 - 33 2-Phenylacetaldehyde (Benzenacetaldehyde) 1050 1.8±0.90 - 1.50±1.22 - 34 (E)-Oct-2-enal 1063 0.49±0.18 - 0.76±0.22 - 35 1-Phenylethanone (Acetophenone) 1072 - - 0.55±0.08 - 36 Nonan-2-one 1091 0.66±0.06 - 0.34±0.00 - 37 Nonan-3-one 1091 - - 0.42±0.00 - 38 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one (Fenchone) 1096 - - 0.34±0.00 - 39 3,7-Dimethylocta-1,6-dien-3-ol (Linalool) 1102 - - 1.16±0.00 - 40 Nonanal 1102 - - - 2.41±0.13 41 2,6-Dimethylocyclohexan-1-ol 1110 - 0.97±0.21 - 1.78±0.15	32	Phenylmethanol (Benzyl alcohol)	1042	1 61+0 15	14 78+1 62		18 90+0 46
34 (E)-Oct-2-enal 1063 0.49±0.18 - 0.76±0.22 - 35 1-Phenylethanone (Acetophenone) 1072 - - 0.55±0.08 - 36 Nonan-2-one 1091 0.66±0.06 - 0.34±0.00 - 37 Nonan-3-one 1091 - - 0.42±0.00 - 38 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one (Fenchone) 1096 - - 0.34±0.00 - 39 3,7-Dimethylocta-1,6-dien-3-ol (Linalool) 1102 - - 1.16±0.00 - 40 Nonanal 1102 - - 2.41±0.13 41 2,6-Dimethylcyclohexan-1-ol 1110 - 0.97±0.21 - 1.78±0.15	33	2-Phenylacetaldehyde (Benzenacetaldehyde)	1050	1 8+0 90	_	1 50+1 22	_
35 1-Phenylethanone (Acetophenone) 1072 - - 0.55±0.08 - 36 Nonan-2-one 1091 0.66±0.06 - 0.34±0.00 - 37 Nonan-3-one 1091 - - 0.42±0.00 - 38 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one (Fenchone) 1096 - - 0.34±0.00 - 39 3,7-Dimethylocta-1,6-dien-3-ol (Linalool) 1102 - - 1.16±0.00 - 40 Nonanal 1102 - - 2.41±0.13 41 2,6-Dimethylcyclohexan-1-ol 1110 - 0.97±0.21 - 1.78±0.15	34	(<i>F</i>)-Oct-2-enal	1063	0 49+0 18	_	0.76+0.22	_
36 Nonan-2-one 1091 0.66±0.06 - 0.34±0.00 - 37 Nonan-3-one 1091 - - 0.42±0.00 - 38 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one (Fenchone) 1096 - - 0.34±0.00 - 39 3,7-Dimethylocta-1,6-dien-3-ol (Linalool) 1102 - - 1.16±0.00 - 40 Nonanal 1102 - - 2.41±0.13 41 2,6-Dimethylcyclohexan-1-ol 1110 - 0.97±0.21 - 1.78±0.15	35	1-Phenylethanone (Acetonhenone)	1072	-	_	0.55+0.08	_
37 Nonan-3-one 1091 - - 0.42±0.00 - 38 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one (Fenchone) 1096 - - 0.34±0.00 - 39 3,7-Dimethylocta-1,6-dien-3-ol (Linalool) 1102 - - 1.16±0.00 - 40 Nonanal 1102 - - 2.41±0.13 41 2,6-Dimethylcyclohexan-1-ol 1110 - 0.97±0.21 - 1.78±0.15	36	Nonan-2-one	1091	0.66+0.06	_	0 34+0 00	_
38 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one (Fenchone) 1096 - - 0.34±0.00 - 39 3,7-Dimethylocta-1,6-dien-3-ol (Linalool) 1102 - - 1.16±0.00 - 40 Nonanal 1102 - - 2.41±0.13 41 2,6-Dimethylcyclohexan-1-ol 1110 - 0.97±0.21 - 1.78±0.15	37	Nonan-3-one	1091	_	_	0.42+0.00	_
39 3,7-Dimethylocta-1,6-dien-3-ol (Linalool) 1102 - - 1.16±0.00 - 40 Nonanal 1102 - - - 2.41±0.13 41 2,6-Dimethyloctol-1-ol 1110 - 0.97±0.21 - 1.78±0.15	38	1 3 3-Trimethylbicyclo[2 2 1]bentan-2-one (Fenchone)	1096	_	_	0.34+0.00	_
40 Nonanal 1102 - - - 2.41±0.13 41 2,6-Dimethylcyclohexan-1-ol 1110 - 0.97±0.21 - 1.78±0.15	39	3 7-Dimethylocta-1 6-dien-3-ol (Linalool)	1102	_	_	1 16+0 00	_
41 2,6-Dimethylcyclohexan-1-ol 1110 - 0.97±0.21 - 1.78±0.15	40	Nonanal	1102	_	_	_	2 41+0 13
	41	2 6-Dimethylcyclohexan-1-ol	1110	_	0 97+0 21	_	1 78+0 15
42 4-Methyl-1-(1-methylethyl)-bicyclo[3,1,0]hexan-3-one (β-Thuione) 1110 – – 0.34+0.00 –	42	4-Methyl-1-(1-methylethyl)-bicyclo[3.1.0]hexan-3-one (B-Thuione)	1110	_	_	0.34+0.00	_
43 2-Phenylethanol (Phenethyl alcohol) 1118 1.82+0.74 – 1.41+0.00 –	43	2-Phenylethanol (Phenethyl alcohol)	1118	1.82+0.74	_	1.41+0.00	_
44 Dodecane 1203 – – – 1.00+0.26	44	Dodecane	1203	_	_	_	1.00+0.26
45 Dodec-2-ene 1213 1.44±0.05	45	Dodec-2-ene	1213	_	_	_	1.44±0.05
46 2.6.6-Trimethylcyclohexene-1-carbaldehyde (8-Cyclocitral) 1226 – 0.77±0.18 – – –	46	2.6.6-Trimethylcyclohexene-1-carbaldehyde (B-Cyclocitral)	1226	_	0.77±0.18	_	_
47 (2F)-3.7-Dimethylocta-2.6-dienal (G-Citral) 1243 – 1.65+0.16 – –	47	(2 <i>F</i>)-3.7-Dimethylocta-2.6-dienal (β-Citral)	1243	_	1.65+0.16	_	_
48 1H-Indole 1292 - 0.95±0.10 - 1.56±0.79	48	1H-Indole	1292	_	0.95±0.10	_	1.56±0.79
49 Undecan-2-one 1294 0.55+0.07	49	Undecan-2-one	1294	0.55+0.07	_	_	_
50 4-(2,6,6-Trimethylcyclohexen-1-yl)but-3-en-2-one (β-lonone) 1485 – 0.88±0.00 0.88±0.00 0.65±0.12	50	4-(2,6,6-Trimethylcyclohexen-1-vl)but-3-en-2-one (B-lonone)	1485	_	0.88±0.00	0.88±0.00	0.65±0.12
51 Pentadecane 1503 1.86±0.08 – 1.34±0.16 0.51±0.06	51	Pentadecane	1503	1.86±0.08	_	1.34±0.16	0.51±0.06
52 2,4-Di <i>tert</i> -butylphenol 1513 – – 0.89±0.00 –	52	2,4-Di <i>tert</i> -butylphenol	1513	_	_	0.89±0.00	_
53 Hexadecane 1602 0.81±0.01 1.15±0.18 1.20±0.25 2.44±0.27	53	Hexadecane	1602	0.81±0.01	1.15±0.18	1.20±0.25	2.44±0.27
54 Heptadec-8-ene 1680 – – 0.74±0.28 –	54	Heptadec-8-ene	1680	_	_	0.74±0.28	_
55 Heptadecane 1703 22.51±0.36 59.85±2.48 39.37±6.66 24.03±0.89	55	Heptadecane	1703	22.51±0.36	59.85±2.48	39.37±6.66	24.03±0.89

* SD is the standard deviation of sample triplicate; ${\sf RI-retention}$ index.

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(Table 1, Figure 2). A higher percentage of heptadecane in the dry sample can be attributed to the presence of cyanobacteria living symbiotically with sponges. It has been discovered that the biosynthetic pathway from cyanobacteria consists of the acyl-acyl carrier protein reductase and the aldehyde decarbonylase, which together convert the intermediates of fatty acid metabolism into alkanes and alkenes.^[17] Several other saturated hydrocarbons such as hexadecane and pentadecane were identified in smaller proportions in almost all samples (Table 1).

The second most dominant group of compounds were benzene derivatives (Figure 1). In HS-FrPF higher presence of benzaldehyde was found compared to HS-DrPF (6.9 times, f1; 2.0 times, f2) (Figure 2). As already explained in the previously published research^[18–20] the loss of benzaldehyde during air drying could be due to its high volatility. On the other hand, benzyl alcohol percentage increased in the dry samples (9.2 (f1) – 18.9 (f2) times). Phenylpropane derivatives are derived from phenylalanine with the side-chain shortened by two carbon atoms which can take place β -oxidatively or non-oxidatively.^[21]

The compounds containing nitrogen showed similar abundance when analysed with f1 (8.30 %, HS-FrPF; 7.94 %, HS-DrPF), but when analysed with f2 they were 15.3 times higher in HS-DrPF (1.50 %, HS-FrPF; 22.90 %, HS-DrPF) (Figure 1). The volatile amine, *N*,*N*-dimethylmethanamine (trimethylamine) has been frequently used as a freshness parameter of marine organisms. Trimethylamine is formed from trimethylamine oxide (TMAO) as the result of the action of bacteria that cause spoilage,^[22] which may explain the higher percentage of this amine in dry samples (2.1 (f1) – 19.1 (f2) times). The aromatic heterocyclic compound pyridine was found in all samples and its percentage decreased 1.0 (f2) – 1.7 (f2) times after air-drying. Pyridine derivatives are often part of biomolecules in marine sponges such as alkaloids.^[23]

Among terpenes, *p*-cymene, eucalyptol, fenchone, linalool, β -thujone and β -citral were detected in a low percentage. Other compounds such as norisoprenoids, organohalogen compounds and fatty acid derivatives were detected with minor abundance in the total headspace composition.

Composition of the VOCs Obtained by Hydrodistillation

Analysis of the VOCs in the hydrodistillate resulted in 88.53 % in FrPF (HD-FrPF) and 77.02 % in DrPF (HD-DrPF) of the total identified compounds (Table 2).

In both samples, the group of aliphatic compounds predominated with 44.99 % in HD-FrPF and 36.67 % in HD-DrPF (Figure 3). Oct-1-en-3-ol, oxylipin known as global metabolome that induces the defence of marine invertebrates and algae,^[15] had the greatest abundance in HD-FrPF. It decreased 30.1 times after drying probably because of its high volatility (Figure 4). Nine more oxylipins were detected and identified (Table 2). Heptadecane, as the second most abundant aliphatic compound in HD-FrPF, was present with lower abundance than in the headspace of the samples extracted by HS-SPME (Figure 4).

The second most represented group of identified compounds was benzene derivatives (17.27 %, HD-FrPF; 12.09 %, HD-DrPF) (Figure 3) with diisobutyl phthalate as the dominant compound (8.44 %, HD-FrPF; 1.80 %, HD-DrPF) (Figure 4). Di-*n*-phthalates were found in the marine sponges *Cinachyrella cavernosa*^[24] and *Halidcondria* sp.,^[25] and their presence in sponges potentially originates from cyanobacteria on sponges. Two more benzene derivatives in higher abundance were identified: 1,4-xylene (2.87 %, HD-FrPF; 2.37 %, HD-DrPF) and benzaldehyde (2.43 %, HD-FrPF; 2.36 %, HD-DrPF).

In HD-FrPF 15.06 % of the total identified compounds belonged to the group of fatty acids and derivatives (Figure 3). In HD-DrPF, the portion of this group decreased 41.1 times. Two hexadecanoic acid esters, methyl (*Z*)-hexadec-7enoate (3.77 %) and ethyl (*E*)-hexadec-9-enoate (3.66 %), were identified in HD-FrPF with higher abundance, but were not detected in HD-DrPF (Figure 4). The reason for fatty acid esters decrement after the drying may be oxidation reactions and lipid decomposition that can occurred during the drying.

Among the compounds containing sulphur, dimethyl trisulphide was quantitatively important, and its proportion increased after the drying (5.31 %, HD-FrPF; 7.50 %, HD-DrPF) (Figure 3). It was also the most abundant compound in HD-DrPF. Dimethyl trisulphide, along with other compounds, could be responsible for the strong, unpleasant smell that this sponge produced. The role of sulphur compounds in marine sponges is probably the defence against predators.^[26,27]

The second most abundant compound in HD-DrPF was 1H-indole with 6.00 % (Figure 4). The indoles alkaloids are broadly present in the metabolism of marine organisms, especially sponges.^[28] Indole alkaloids containing a benzopyrrole skeleton exhibit antibacterial, antimicrobial, cytotoxic and antineoplastic properties.^[29,30]

Carotenoid degradation products, C₁₃-norisoprenoides, were more abundant in the hydrodistillate of the dry sample. β -lonone increased 3.6 times after the drying, and β -cyclohomocitral, was detected only in the dry sample. Chlorophyll derivatives phytane and hexahydrofarnesyl acetone (phytone) were found. After the drying, their content increased, probably due to the degradation of chlorophyll.^[31]



■ HS-FrPF (f1) ■ HS-DrPF (f1) ■ HS-FrPF (f2) ■ HS-DrPF (f2)

Compounds

containing

sulphur

Terpenes

Other

Compounds

containing

nitrogen

Aliphatic

compounds

Benzene

derivatives

Figure 1. The volatile organic compounds of *P. ficiformis* extracted by headspace solid-phase microextraction (HS-SPME), analysed by gas chromatography-mass spectrometry (GC-MS) and sorted by structural groups. Extraction by DVB/CAR/PDMS fibre (f1): HS-FrPF (f1) – fresh *P. ficiformis*; HS-DrPF (f1) – air-dried *P. ficiformis*. Extraction by PDMS/DVB fibre (f2): HS-FrPF (f2) – fresh *P. ficiformis*; HS-DrPF (f2) – air-dried *P. ficiformis*.



Figure 2. The most abundant compounds from *P. ficiformis* samples extracted by HS-SPME and analysed by GC-MS. The volatile organic compounds of *P. ficiformis* extracted by headspace solid-phase microextraction (HS-SPME), analysed by gas chromatography-mass spectrometry (GC-MS) and sorted by structural groups. Extraction by DVB/CAR/PDMS fibre (f1): HS-FrPF (f1) – fresh *P. ficiformis*; HS-DrPF (f1) – air-dried *P. ficiformis*. Extraction by PDMS/DVB fibre (f2): HS-FrPF (f2) – fresh *P. ficiformis*; HS-DrPF (f2) – air-dried *P. ficiformis*.



N	Compaund		Area (%) ± SD*	
NO.	Compound	KI -	V	VI
1	2-Methyl-1H-pyrrole	750	0.32±0.07	0.16±0.10
2	Furan-2-carbaldehyde (Furfural)	830	0.16±0.04	0.16±0.09
3	(E)-Hex-2-enal	857	0.39±0.01	0.41±0.10
4	4-Methyloctane	863	-	0.03±0.03
5	Ethylbenzene	868	1.00±0.01	0.67±0.03
6	1,4-Xylene (<i>p</i> -Xylene)	878	2.87±0.15	2.37+-0.08
7	(3E,5Z)-Octa-1,3,5-triene (Fucoserratene)	879	0.19±0.02	_
8	Cycloocta-1,3,5,7-tetraene	880	-	0.08±0.03
9	Heptan-2-one	889	0.71±0.04	0.28±0.07
10	Styrene	890	0.10±0.00	-
11	1,2-Xylene (o-Xylene)	894	-	0.61±0.03
12	Nonane	900	-	0.58±0.01
13	(Z)-Hept-4-enal	901	2.48±0.16	-
14	Heptanal	902	0.61±0.01	0.22±0.07
15	3-(Methylsulfanyl)propanal (Methional)	906	0.19±0.01	0.22±0.07
16	Benzaldehyde	961	2.43±0.16	2.38±0.68
17	(Methyltrisulfanyl)methane (Dimethyl trisulfide)	972	5.31±0.10	7.50±2.34
18	Heptan-1-ol	975	0.30±0.01	-
19	Oct-1-en-3-ol	982	8.65±0.58	0.29±0.04
20	Octan-2,5-dione	983	-	0.28±0.09
21	Phenol	984	-	0.22±0.01
22	Octan-2,3-dione	987	0.18±0.05	-
23	Benzonitrile	986	-	0.20±0.01
24	2,4,6-Trimethylpyridine	987	-	0.45±0.01
25	Octan-3-one	988	1.60±0.03	-
26	Octan-2-one	992	0.38±0.03	-
27	Octanal	1005	0.18±0.01	0.12±0.01
28	1-Methylpyrrole-2-carbaldehyde	1010	0.25±0.00	0.17±0.03
29	(<i>E,E</i>)-Hepta-2,4-dienal	1012	0.07±0.00	-
30	Bis(1-Methylethyl) disulphide (Diisopropyl disulphide)	1016	-	0.05±0.05
31	2-Ethylhexan-1-ol	1029	0.13±0.00	0.12±0.02
32	1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane (Eucalyptole)	1035	0.26±0.08	-
33	Phenylmethanol (Benzyl alcohol)	1040	0.59±0.20	0.61±0.07
34	2-Phenylacetaldehyde (Benzenacetaldehyde)	1050	1.17±0.30	1.75±0.66
35	2-Methyldecane	1061	0.15+-0.02	-
36	(E)-Oct-2-enal	1063	0.66±0.06	0.22±0.03
37	1-Phenylethanone (Acetophenone)	1066	-	0.40±0.10
38	(<i>E</i>)-Oct-2-en-1-ol	1071	2.12±0.07	-
39	Octan-1-ol	1074	-	0.03±0.01
40	Octylcyclopropane	1075	2.65±0.18	0.11±0.00
41	(<i>E,E</i>)-Octa-3,5-dien-2-one	1083	0.33±0.05	-
42	Nonan-2-one	1091	0.10±0.02	0.20±0.04
43	Nonanal	1102	0.15±0.01	0.32±0.07
44	3,7-Dimethylocta-1,6-dien-3-ol (Linalool)	1104	0.40±0.01	0.45±0.12
45	2,6-Dimethylcyclohexan-1-ol	1110	0.17±0.03	0.24±0.05
46	2-Phenylethanol (Phenethyl alcohol)	1117	0.28±0.15	-
47	Phenylpropan-2-one (Phenylacetone)	1124	-	0.10±0.01
48	1-(4-Methylcyclohex-3-en-1-yl)ethanone	1130	-	0.34±0.05
49	1,7,7-Trimethylbicyclo[2.2.1]heptan-2-one (Camphor)	1139	0.12±0.04	0.04±0.04
50	(<i>E,Z</i>)-Nona-2,6-dienal	1156	1.02±0.10	0.45±0.18
51	(Z)-Non-2-en-1-al	1162	0.44±0.04	0.28±0.11
52	1,7,7-Trimethylbicyclo[2.2.1]heptan-2-ol (Borneol)	1167	-	0.03±0.03
53	Decan-2-one	1194	0.15±0.00	0.28±0.02
54	Decanal	1200	0.50±0.02	0.33±0.03
55	1-Methoxy-4-(prop-2-en-1-yl)benzene (Estragole)	1201	-	0.17±0.03
56	(3Z,5Z)-2,6-Dimethylocta-3,5,7-trien-2-ol	1209	-	0.20±0.02
57	2-Methoxy-1-methyl-4-(1-methylethyl)-benzene (Carvacrol methyl ether)	1250	0.09±0.00	-

Table 2. The VOCs from *P. ficiformis* isolated by HD and analysed by GC-MS: (VI - HD of fresh *P. ficiformis*, VII - HD of air-dried *P. ficiformis*).SD is standard deviation of sample triplicate; RI – retention index

* SD is the standard deviation of sample triplicate; ${\sf RI-retention}$ index.



Table 2. Continued.

no. Collingenia no. V V 56 212,6,6 TrinetHybeshern 1 (jacriddehyse (f Cyclohomachia)) 101 - 0.030,0.01 56 0.7,6,1,1-17restHybeshern 1275 0.324,0.01 - 61 1.11+ridde 1207 0.324,0.01 - 62 0.7,6,1,1-17restHybeshare 1308 0 0.224,0.02 63 0.10 releanal 1308 0 0.224,0.02 64 0.10 releanal 1308 0.40,0.02,0.02 - 65 0.2C41/2 unetHyberoanotats (CapyM) inductyrate) 1348 0.442,0.02 - 66 Phoromotheracer (Diphery ether) 1355 0.252,0.00 0.252,0.00 70 0.35 Methydecanol card 1417 - 0.276,0.02 71 1.(5) f.(10 Dimethymelones 3,5 dim 2 one ([() renarylaeribore] 1475 - 0.422,0.00 73 Doddecan-1 on 1468 - 0.124,0.00 - 74 1.(5) f.(1,0 Dimethyberofee, 5-4,0.00 1485 0.944,0.00 -	No	Compound	DI.	Area (9	%) ± SD*
S6 2.12,6.6 Trimethylophene, Muserialdehydi (K.yolobanoutiral) 1261 - 0.23,0.0 59 Dec.2 entl 1273 3.32,0.00 - 60 2.6.1.1*methylophene 1275 3.32,0.00 - 61 1.1.1*methylophene 1292 0.52,0.02 60,002,83 62 1.2.becylourane 1397 0.228,0.01 - 63 Undocani 1398 - 0.122,0.02 64 O.tyl_amethylopeanota (Copyl klobutytat) 1388 0.228,0.02 - 65 O.tyl_amethylopeanota (Copyl klobutytat) 1398 0.228,0.02 - 66 O.tyl_amethylopeanota (Copyl klobutytat) 1398 0.228,0.02 - 67 Dodecan-bore 1397 - 0.228,0.02 - 70 Dodecan-bore 1397 - 0.228,0.02 - - 0.428,0.03 - - 0.428,0.03 - - 0.428,0.03 - - 0.428,0.03 - - 0.428,0.03 - -	NO.	Compound	RI	V	VI
9 DBc2 en 1-d 175 3.220.00 60 A.B.I.Finethylkobcane 1075 0.520.02 61 Undersand 108 0.174.00 62 O.C.Y.J. Composition (Composition (Compositant) (Composition (Composition (Comp	58	2-(2,6,6-Trimethylcyclohexen-1-yl)acetaldehyde (β-Cyclohomocitral)	1261	-	0.20±0.03
60 2,6,11 (monthlybiodecane) 172 0.338.000 - 61 2,600/00137 1307 0.288.001 - 62 0.400/00137 1308 - 0.2124.002 63 0.400/00137 1308 0.2124.002 - 64 0.0121.00137 1308 0.288.001 0.0124.002 65 0.0121.00137 1308 0.288.001 0.0124.002 66 0.0240.003 0.0240.003 0.0240.003 0.0240.003 71 0.0260.001 0.0250.001 0.0250.001 0.0250.001 72 0.0260.011 1408 - 0.0240.003 73 0.00600000 1408 - 0.0240.003 74 1.010100000000000 1408 - 0.0240.003 75 1.4401.011 1.010 0.0240.003 1.0240.001 76 1.651.000 1.0100 0.0240.003 1.0240.001 76 1.651.000 1.0100 0.0240.003 1.0240.001 76 <	59	Dec-2-en-1-ol	1273	1.32±0.10	-
61 114midale 1370 0.250.001 - 62 0.2000rane 1360 0.280.001 - 63 0.000rane 1360 0.390.002 - 64 0.46.000recthylobacture 1340 0.480.003 0.420.007 65 0.000rectan-3-one 1340 0.280.003 0.270.003 66 0.000rectan-3-one 1340 0.290.001 0.376.002 71 0.000rectan-3-one 1340 0.290.001 0.376.002 72 0.521.0.000recthylundece 5.9.40m-2.one (£) Geranylucetone) 1442 0.290.001 0.376.002 72 1.344.014/bit-56-art-1/g/lost-1-ar-2-one (£) Geranylucetone) 1445 0.290.001 - 0.428.001 73 1.344.014/bit-56-art-1/g/lost-1-ar-2-one (£) Geranylucetone) 1445 0.480.00 - - 0.428.001 74 1.344.014/bit-56-art-1/g/lost-1-ar-2-one 1467 - 0.1240.01 - - 0.428.001 - - 0.428.001 - - 0.428.001 - - 0.428.001 - - 0.428.001 - - 0.428.001	60	2,6,11-Trimethyldodecane	1275	0.33±0.00	-
i 2.Decydoriane 1367 0.28.00 i 0.10.002 0.12.002 0.12.002 i 0.44.00 i 0.001/2.methylapoganot (caryl) kobulyrate) 1348 0.448.002 i Dodacan-3-one 1347 0.28.002 0.272.003 i Phenophenese (liphenyl ether) 1368 0.28.002 0.278.003 i Dodacan-3-one 1407 0.290.002 i Scholarshieless-3-den-2-one (l-foranylaceton) 1442 0.190.00 0.591.00 i Scholarshieless-3-den-2-one (l-foranylaceton) 1452 0.901.00 0.591.00 i Scholarshieless-3-den-2-one (l-foranylaceton) 1453 0.400.00 0.591.00 i Scholarshieless-3-den-2-one 1473 0.401.00 0.191.00 i Scholarshieless-3-den-2-one 1497 0.401.00 0.191.00 i Scholarshieless-3-den-2-one 1501 0.410.00 0.191.00 i Scholarshieless-3-den-2-one 1531 <	61	1H-Indole	1292	0.52±0.02	6.00±0.83
63 Undecanal 1388 0.12:002 64 0.46-0inerthylopanotek (Caprylitobaryzte) 1348 0.44:003 65 Obdecan-2-one 1349 0.25:003 0.02:003 67 Obdecan-2-one 1349 0.25:003 0.02:000 68 Phenoxybernzen (Diphenyl ether) 1429 0.117:0.12 0.02:000 70 Obdecan-2-one (Caprylitobaryzte) 1452 0.19:0.00 0.05:0.01 71 (E)-6.10-Obdec4-m-2-one (B-Oranylicatone) 1458 0.19:0.00 73 Obdeca-2-one (Caprylitobaryzte) 1458 0.41:0.00 74 1.4Methyl-6.5-en-1/olpothae-2-ane (B-Oranylicatone) 1458 0.44:0.00 75 1.4Methyl-6.5-en-1/olpothae-2-ane (B-Oranylicatone) 1458 0.44:0.00 75 1.4Methyl-6.5-en-1/olpothae-2-ane (B-Oranylicatone) 1458 0.44:0.00 76 1.4Methyl-6.5-en-1/olpothae-2-ane (B-Orany) 14:0:0:0:0 0.0:0:0:0 76 1.4Methyl-6.5-en-1/olpothae-2-ane (B-Orany)	62	2-Decyloxirane	1307	0.28±0.01	-
64 0.4.6.0 methydocacane 135 0.340.00 65 0.0cty/zmethydopacane(zapryl insburytze) 138 0.240.00 0.242.005 75 0.0cto/zmethydopacane(zapryl insburytze) 1385 0.270.003 0.242.005 76 0.0cto/zmethydinecacane 1376 0.206.00 0.266.00 76 0.0cto/zmethydinecacane 1407 0.266.00 71 (E) 0.0cto/zmethydinecacas.5.9.der -2.one (E) Geranylsectone) 1438 0.262.00 73 0.0cto/zmethydinecacas.5.9.der -2.one (E) Geranylsectone) 1438 0.262.00 74 0.10cto/zmethydinecaca 1438 0.262.00 75 1.Methyl 4.16.methyldinecaca 1438 0.262.00 76 (E) 4.2.0.6. Tindican-2-one 1438 0.240.00 76 0.24.00 0.250.03 76 0.24.00 0.250.03 0.250.03 76 1.44.44/04.7.11.450.04 0.0410.01 0.250.01	63	Undecanal	1308	-	0.12±0.02
6 Octyl 2-methynopanoat (Capvyl Jobutyrate) 1348 0.424003 0.424003 67 Obdecan-3-one 1387 0.724003 68 Phenosoberone (Dipheny ether) 1387 0.424003 70 Shehryldecanic acid 1407 1.1720.12 0.054003 71 (ES)-6,10-Dimethyldneces-5-Anel-Cale (Folearnylacebone) 1468 - 0.254003 72 (.1)-Obdec-8-en-1-ol 1468 - 0.194010 73 Dodocan-1-ol 1468 - 0.194010 74 Obdocan-1-ol 1468 - 0.194010 75 1.4-Methyl-4-Ener-9/Qitc/Jachez-1-dien (/Curcurene) 1473 0.40100 0.3810.18 76 (.1)-Methyl-4-Ener-1/Qitc/Jachez-1-diene (/Curcurene) 148 - 0.1940.19 76 (.1)-Methyl-4-Ener-1/Qitc/Jachez-1-diene (/Curcurene) 148 0.402000 - 77 Tridacanal 151 0.452001 - 0.1940.19 78 A.2-Methyl-4-Ener-1/Qitc/Jachez-1-diene (/Curcurene) 1531 0.452001 -	64	4,6-Dimethyldodecane	1325	0.39±0.02	-
66 Dodecan-some 1340 1.240.03 0.2420.03 67 Dodecan3-some 1395 0.350.00 0.2420.03 68 Phenoxybarnzne (Diphenyi ether) 1395 0.350.00 0.2420.03 70 JAMethyldecanoic add 1409 1.170.01 0.0370.01 71 (5)6-0.10-00methylundeca-3,5-dien-2-one (U)-0-00methylundeca-3,5-dien-2-one (U)-0-00methylundeca-3,5-dien-2-one (U)-0-00methylundeca-3,5-dien-2-one (S-innone) 1468 1.0480.00 73 Dodecan-1-ol 1473 0.520.00 - 1.350.01 74 (I-1)-04-12,6-6-Trientyllund-2-en-1-ol 1473 0.520.00 - 1.350.01 75 I-1-Methyl-4-(6-methyllund-2-en-1-ol 1473 0.520.00 - 1.350.01 3.380.01 76 I-1-Methyl-4-(6-methyllund-2-en-1-ol 1470 0.420.00 - - 1.350.01 - 77 I-1-Methyl-4-(6-methyllund-2-en-1-ol 1470 - 0.350.01 - - 0.550.01 - - 0.550.01 - 0.550.01 - 0.550.01	65	Octyl 2-methylpropanoate (Caprylyl isobutyrate)	1348	0.44±0.02	-
67 Dodecan 3-one 1387 6272003 68 Phenoxoberance (Dyheny ether) 1387 0.242003 70 3-Methylacka acid acid 1403 1.1720.12 0.5780.03 71 (\$26) 6.10 0imethylacka acid acid 1417 0.2640.03 73 Dodecan-1-ol 1468 0.2840.01 74 (\$6) Dodec 2-en-3-ol 1473 0.20200 75 1.Methyl-4(Erschapthylechosz-1, 3-dine (r.Curcumen) 1473 0.4820.03 76 (\$6) A-2.5.5.000 1483 0.4820.03 78 Amethylackance 2-one 1593 0.4820.03 78 Amethylackance 2-one 1503 0.4820.03 78 Amethylackance 2-one 1503 0.4820.03 78 Amethylackance 2-one 1503 0.4520.01 1.2124.063 78 Amethylackance 2-one 1503 0.4520.01 1.2124.063 79 Amethylackance 1503	66	Dodecan-2-one	1349	0.28±0.03	0.42±0.05
66 Phenoxyberzene (Diphery letter) 1596 0.000 0.256.02 69 Dodecanal 117 0.256.02 71 (£5)-5.10-Dimethylundecs-5.9-dien-2-one ([£)-Geranylacetone) 1462 0.0529.00 72 (£)-Dodecs-8n-1-ol 1468 - 1.0480.00 73 Dodecan-1-al 1468 - 0.0420.00 74 (£)-Odec 2-en -0 1473 0.6220.00 - 75 1.Methyl-4.5-methylpethyl-sen-2-one (§-Lonore) 1478 - 0.0420.00 76 (£)-4/2.6.6-Trimtylpetholoc-2-one (§-Lonore) 1487 - 0.550.03 78 Prendaccane 1503 0.448.003 - 79 2.25 Ditert butylphenol 1514 - 0.550.03 81 0.14-monodocane 1513 0.438.00 - 82 1.4-fu-hydray-3-methorypherylprepan -2one (Suiacyl acetone) 1514 - 0.7040.03 82 1.4-fu-hydray-3-methorypherylprepan -2one (Suiacyl acetone) 1513 0.448.00 - 83 0.1414.00000 <td>67</td> <td>Dodecan-3-one</td> <td>1387</td> <td>-</td> <td>0.27±0.03</td>	67	Dodecan-3-one	1387	-	0.27±0.03
end Dodecand 1400 1.740.12 0.0700.03 71 (5f)-6,10-Dimethylundeca-5,9-dimet-2-one (l/E)-Geranylacetone) 1452 0.19:0.00 0.59:0.01 72 (c/E)-0.06-2-en-1.01 1468 - 0.48:0.00 73 Dodecant-1.01 1473 0.62:0.00 - 74 Matthyl-14-(E-nethyllyndec-2-en-1.91) 1473 0.62:0.00 - 76 1-Matthyl-4-(E-nethyllyndec-2-en-1.91) 1473 0.62:0.00 - 76 (c/E)-4.(2.6.6-Trimethyllyclobexen-2-one (B-loone) 1485 0.69:0.02 - 77 Tridecanal 1511 1.33:0.018 1.22:0.018 78 Pertadecane 1503 0.69:0.02 - 79 C-Bromododecane 1514 - 0.55:0.01 71 Tridecanal 1514 0.43:0.01 1.96:0.02 74 Tridecanal-1.610-(Finithyllyndecan-2.610-(Finithyllyndecan-1.610-(Finithyllyndecan-1.610-(Finithyllyndecan-1.610-(Finithyllyndecan-1.610-(Finithyllyndecan-1.610-(Finithyllyndecan-1.610-(Finithyllyndecan-1.610-(Finithyllyndecan-1.610-(Finithyllyndecan-1.610-(Finithyllyndecan-1.610-(Finithyllyndecan-1.610-(Finithyllyndec	68	Phenoxybenzene (Diphenyl ether)	1396	0.25±0.00	0.26±0.02
70 3-Methyldecanck jold 1417 - 0.2650.2 71 (5F)-6,16-Dimethylundeca-5,9-dimethylenylaseteno) 1468 - 0.4860.01 73 Dodecan-1-ol 1468 - 0.4860.01 74 (E)-Dode 2-en 1-ol 1473 0.622.000 - 75 1-Methyl-4-16-methylecyl-5-en 2-yllox-3-hosen_13-dine (µCurcumene) 1475 - 0.1920.03 76 (E)-4.2,6-G ⁻ methylecyl-5-en 2-yllox-3-methylecol-sene (J-lonone) 1475 - 0.1920.03 70 Pentadecane 1505 0.4940.00 - - 70 Pentadecane 1505 0.4940.00 - - 71 Tridecanal 1511 1.3840.16 1.2240.05 72 1.41440/doxy-3-methoxylenylenyla 2-ne (Golasyl actone) 151 0.4540.01 - 73 1.44440/doxy-3-methoxylenylenyla 2-ne (Golasyl actone) 153 0.4540.01 1.950.03 74 Tridecanel 2-ne 156 0.1340.02 1.960.03 - 0.2940.03 74 Heradecane	69	Dodecanal	1409	1.17±0.12	0.97±0.04
1 (SF)-6,10-Dimethylundera-5,8-dim-2-one ((J-Garanylacetone) 1452 0.1940.00 73 Obdetan-1-ol 1468 - 0.2940.00 74 (-)-Dodec 2-en-1-ol 1473 0.6940.00 - 75 1-Abethyl-4-(-E-methylherbi-5-en-2-ulg)(c-Durcar) 1475 - 0.1940.10 76 (-)-Abethyl-4-(-E-methylherbi-5-en-2-une (J-Lonone) 1485 0.4940.05 78 - 1360.04 - 3.860.18 78 - Pentadecane 1503 0.4940.05 79 - 2.8000.00000000000000000000000000000000	70	3-Methyldecanoic acid	1417	-	0.26±0.26
2 (2) Dode: 2 en : l ol 1468 - 0.480.01 74 Dode: 2 en : l ol 1468 - 0.120.03 75 1.4461/4-LG-mth/hept-S-en 2-/lpc/chose-1.3-dien (r_Curcumene) 1475 - 0.120.03 76 (£)-4.2,6.6.1'mth/hept-S-en 2-/lpc/chosen-1.3-dien (r_Curcumene) 1475 - 0.120.03 78 Pentadecane 1505 0.448.00 - 78 Pentadecane 1505 0.484.00 - 79 2.5.0'Dirrt-Mu/phenol 151 0.455.00 - 71 Tridecana 2-one 1531 0.455.00 - 0.702.03 74 1.444/ydrowi-3-methowyben/lpropar-2-one (Guiakyl actore) 1531 0.455.00 - 0.702.03 74 Tridecana 2-one 1579 0.312.002 0.312.002 0.312.002 75 Tridecana-1.01 156 0.320.012 1.480.01 - 76 Tridecanal 169 0.436.002 1.707.02 76 Tridecanal 160 0.436.002 0.70	71	(5E)-6,10-Dimethylundeca-5,9-dien-2-one ((E)-Geranylacetone)	1452	0.19±0.00	0.59±0.01
73 Dodecan-1.01 1468 1.202.03 74 (F)-Dodec-2en-10 1473 0.6234.00 0.6234.00 75 I-Methyl-4-(6-methylhept-Sen-2-yllovlohea-1,3-diene (y-Curcumene) 1485 0.484.005 0.3840.03 76 (E)4-4(2,6,6-Trimethylovloheae-1,3-diene (y-Curcumene) 1485 0.484.005 77 Tridecana-2-one 1503 0.484.005 78 O-Artomododecane 1503 0.484.005 79 Q-Stromododecane 1514 0.554.003 78 1-4(4-Hydrox)-3-methoxylhenyllopan-2-one (Guiacyl acetone) 1514 0.702.003 74 Tridecana-2-one 1559 0.304.015 1.184.004 74 Tridecane-1.610 (Neroidol) 1544 0.304.015 1.184.004 74 Tridecane-1.610 (Neroidol) 1.294.017 1.394.003 1.184.004 75 Tridecane-1.610 (Neroidol) 0.455.002 1.074.017 1.394.003 76 Hexadecane 1560 0.455.002 1.074.017	72	(Z)-Dodec-8-en-1-ol	1468	-	0.48±0.01
74 (f)-Dodec-2-en-1-ol 1473 0.622000 - 75 1-Methyl-4-16-methylkopt-S-en-2-yllcyclobkez-1,3-blien (y-Curcumene) 1475 - 0.194.019 76 (f)-4 (2,6,6,7 interthylcyclobkez-1,3-blien (y-Curcumene) 1475 0.494.008 3.840.18 78 Pentadecane 1493 0.48 0.695.002 - 80 Pentadecane 1501 0.695.002 - - 80 Pentadecane 1501 0.458.001 1.965.003 81 1-(4+hydroxy-3-methoxybhernyl)propan-2-one (Guiacyl actotne) 1513 0.458.001 1.965.003 82 1-(4+hydroxy-3-methoxybhernyl)propan-2-one (Guiacyl actotne) 1513 0.458.001 1.980.03 83 1-feradecan-2 one 1569 0.306.015 1.880.04 84 Hexadecane 1569 0.366.015 2.680.06 95 1-(4-kopropyclhenyl)-2-methylpropyl actate 1667 - 0.890.01 96 (/2)-Tetradec-3-en-1-al 1618 0.406.01 - 97 1-(4-kopropyclhenyl)-2-methylpro	73	Dodecan-1-ol	1468	-	1.20±0.03
75 1.Methyl-416-methylkryCohoken-1.globen-al.globena 1.globena 1.g	74	(E)-Dodec-2-en-1-ol	1473	0.62±0.00	-
76 (£)-4(2,6,6-Trimethylopclohenen-1ylbut-3-en-2-one (Å-Inone) 1485 0.944.008 3.3810.18 77 Pentadecane 1503 0.484.005 - 78 Pentadecane 1503 0.484.005 - 79 2-Bromododecane 1501 1.330.016 1.224.005 81 2,5-Ditert-butylphenol 1514 - 0.551.003 82 1.4-Hydroxy-3-methoxynberyljorpan-2-one (Gualacyl acetone) 1531 0.451.001 1.646 83 1.Bromododecane 1552 - 0.702.003 84 (6£)-3,7,11-Trimethyldodeca-1,6,10-trien-3-0 (Nerolidol) 1564 0.342.015 1.880.004 85 Tridecanentrile 1579 0.249.017 1.394.003 87 Tridecanentrile 1592 - 0.249.05 88 Hexadecane 1600 0.451.002 1.072.017 89 Tridecanentrile 1591 0.314.002 0.551.007 91 3.{1-Hydroxy-2 (methylaminojethyllphenol (Phenylephrine) 1666 0.111.002 0.551.007 92 1.{1-Hydroxy-2 (methylaminojethyllphenol (Phenylephrine) 1676	75	1-Methyl-4-[6-methylhept-5-en-2-yl]cyclohexa-1,3-diene (y-Curcumene)	1475	-	0.19±0.19
77 Tridecan 2: one 1497 - 1.361.004 78 Pentadecane 1503 0.481.005 - 79 2.Bromododecane 1505 0.692.002 - 80 Tridecanal 1511 1.338.016 1.224.005 81 2.5.Ditert-butylphenol 1531 0.451.001 1.661.003 82 1.44-Hydroxy-3-methoxypheryl/propan-2-one (Gualacyl acetone) 1531 0.451.001 1.661.003 83 1.Firomododecane. 1557 - 0.701.003 84 (6E)-3.7,11-Trimethyldecaca-1.6,10-trien-3-0 (Neroldol) 1564 0.310.02 0.311.002 85 Tetradecane-2-one 1569 0.300.15 1.881.004 86 Hexadec-1-ene 1579 1.29.0.17 1.381.003 87 Tridecanel 1603 1.581.002 0.651.007 88 Hexadec-1-ene 1679 - 0.510.004 90 Tetradecanel 1667 - 0.450.015 91 3-{1-Hydroxy-2-(methylaminojethyllphon()Phenylephrine) 1666 0.110.002 0.551.007 92 1	76	(E)-4-(2,6,6-Trimethylcyclohexen-1-yl)but-3-en-2-one (β-Ionone)	1485	0.94±0.08	3.38±0.18
79 0.48±005	77	Tridecan-2-one	1497	_	1.36±0.04
79 2-Bromododecane 1505 0.699:002 - 80 Tridecanal 1514 1.38:016 1.240.05 81 3.2.5-Diterb-butylphenol 1514 - 0.55:00.03 82 1.4(4-Hydroxy-3-methowphenylpropan-2-one (Gualacyl acetone) 1531 0.45:00.01 0.31:00.02 83 1.6(6)-3.7,11-Trimethyldodeca-1.6,10.triens-30 (Nerolidol) 1564 0.31:00.02 0.31:00.02 84 (6(6)-3.7,11-Trimethyldodeca-1.6,10.triens-30 (Nerolidol) 1564 0.31:00.02 0.31:00.02 85 Tetradecane-2-one 1579 1.29:01.71 1.39:00.03 86 Hexadeca-1-ene 1592 - 0.29:00.05 87 Tridecanenitrile 1593 3.17:05.02 2.68:00.06 91 3-1:1-Hydroxy-2:(methylamino)ethylprophyl acetate 1667 - 0.55:00.07 92 1.4(4-Isopropylphenyl)-2-methylprophyl acetate 1667 - 0.55:00.07 93 1.20-11-en-1-0 1681 0.40:01.01 - 94 Tetradecanenitrile 1679 - 0.51:0.04 95 1.3-Methyltetradecanal 1681 </td <td>78</td> <td>Pentadecane</td> <td>1503</td> <td>0.48±0.05</td> <td>_</td>	78	Pentadecane	1503	0.48±0.05	_
80 Tridecanal 1511 1.331.016 1.221.005 81 2.5-01tert-bitylphenol 1531 0.451.001 1.966.000 82 1.1-(4-Hydroxy-3-methoxymphorph/lpropan-2-one (Gualacyl acetone) 1552 0.456.001 0.366.005 84 0.661-3,7,11.Trimethyldodeca-1,6,10.trien-3-ol (Nerolidol) 1552 0.450.001 0.318.002 85 Tetradecan-2-one 1559 0.308.015 1.388.004 86 Hexadecane 1660 0.455.002 1.070.070 87 Tridecanentrile 1661 0.455.002 1.070.070 89 O.455.005 1.070.070 0.455.005 1.075.007 90 Tetradecane 1660 0.110.002 0.550.001 91 3.[1-Hydroxy-2-(methylaminojethyljhenol/Phylephrine) 1666 0.111.002 0.551.001 91 3.[1-Hydroxy-2-methylaminojethyljhenol/Phylephrine) 166 0.111.002 0.551.001 92 1.4-Isoprophylphenyl-2-methylaminojethyljhenol/Phylephrine) 1669 0.400.011 - 93 0.21.Phytradecane <td< td=""><td>79</td><td>2-Bromododecane</td><td>1505</td><td>0.69±0.02</td><td>_</td></td<>	79	2-Bromododecane	1505	0.69±0.02	_
81 2,5-Ditert-butylphenol 1514 0.5510.03 82 1-(4-Hydrox)-3-methoxybnerylpropan-2-one (Guaioyl acetone) 1552 - 0.7040.03 84 (6E)-3,7,11-Trimethyldodeca-1,6,10-trien-3-ol (Nerolidol) 1564 0.1310.02 0.3110.02 85 Tetradecan-2-one 1579 0.2940.015 1.1840.04 86 Hexadeca-1-ene 1579 1.2940.17 1.3940.01 87 Tridecanenitrile 1592 - 0.2910.05 88 0.4717 tridec-9-en-1-al 1603 0.5840.06 4.0640.01 90 Tetradec-3-ene 1603 0.114.002 0.5540.07 91 3.14.Hydroxy-2-(methylaminojethylphenol (Phenylephrine) 1667 - 0.4540.15 92 1.2(4-Isoproxyhlephnyl)-zerthylphorpoly acetate 1667 - 0.5140.04 93 (2/2)-Tetradec-3-ene 1687 0.4910.05 - - 94 Pentadecanal 1711 0.6340.01 1.0840.05 - - 95 3.3-Methylheptadecane 1768 0.7340.04 0.8840.05 - - 95	80	Tridecanal	1511	1.33±0.16	1.22±0.05
82 1-(4-Hydroxy-3-methoxyphenyl)propan-2-one (Gualacyl acetone) 1531 0.452.0.01 1.9661.0.99 83 1-Bromododcane 1552 - 0.700.0.3 84 (6F)-3,7,11-Trimethyldodca-1,6,10 (Nerolidol) 1564 0.313.0.0.2 1.184.0.04 85 Tetradecan-2.one 1569 0.304.0.15 1.184.0.04 86 Hexadec-1.ene 1579 1.794.0.17 1.394.0.03 87 Tetradecane 1600 0.452.0.02 1.074.0.07 88 Hexadecane 1600 0.452.0.02 1.074.0.07 89 Tetradecanal 1614 3.170.52 2.680.06 91 3-(1-Hydroxy-2-(methylamino)ethyljpheno)(henylephrine) 1660 0.111.0.02 0.554.0.07 92 1.4(4-Sporpoylpenyl)-2-methylamolylactate 1677 - 0.514.0.04 95 1.3-Methylteradecanae 1678 - 0.514.0.04 96 (2)-Tetrade-1-ene-1-ol 1678 0.534.0.04 0.8840.05 - 97 Heptadecane 1703 5.654.0.2 2.4540.01 - 98 Pentadecanale 1703	81	2,5-Di <i>tert</i> -butylphenol	1514	_	0.55±0.03
1-Bromododecane 1552 - 0.70±0.03 84 (16F)-3,7,11-Trimethyldodeca-1,6,10-trien-3-01 (Nerolidol) 1564 0.13±0.02 0.31±0.02 85 Tetradecan-2-one 1569 0.30±0.015 1.18±0.04 86 Hexadec-1-ene 1579 1.29±0.17 1.39±0.03 87 Tridecane-itrile 1509 - 0.29±0.05 88 Hexadecane 1600 0.45±0.02 1.07±0.07 89 (Z)-Tetradec-9-en-1-al 1603 1.58±0.06 0.45±0.02 91 3-11-Hydroxy-2-cmethylpanolpehyllphenol (Phenylephrine) 1660 0.11±0.02 0.55±0.07 92 1-(4-Isopropylphenyl)-2-methylpropyl acetate 1667 - 0.45±0.15 93 (Z)-Tetradec-11-en-1-ol 1673 - 0.5±0.04 95 1.3+Methyltetradecanal 1681 0.40±0.11 - 96 (Z)-Hetradec-3-ene 1687 0.91±0.06 - 97 Heptadecane 1701 0.5±0.01 - 98 Patadecanal <td< td=""><td>82</td><td>1-(4-Hydroxy-3-methoxyphenyl)propan-2-one (Guaiacyl acetone)</td><td>1531</td><td>0.45±0.01</td><td>1.96±0.09</td></td<>	82	1-(4-Hydroxy-3-methoxyphenyl)propan-2-one (Guaiacyl acetone)	1531	0.45±0.01	1.96±0.09
84 (66)-3,7,11-Trimethyldodeca-1,6,10-trien-3-01 (Nerolidol) 1564 0.13±0.02 0.31±0.02 85 Tetradecan-2-one 1569 0.30±0.15 1.18±0.04 86 Hexadec-1-ene 1579 1.29±0.17 1.39±0.03 87 Tridecanenitrile 1560 0.45±0.02 1.07±0.07 89 (Z)-Tetradec-9-en-1-al 1603 1.58±0.06 4.06±0.01 90 Tetradecanal 1614 3.12±0.52 2.68±0.06 91 3-[1-Hydroxy-2-(methylamio)ethyllphenol (Phenylephrine) 1660 0.11±0.02 0.55±0.07 92 1-44±0spropylphenyl-2-methylpropyl acetate 1667 - 0.45±0.15 93 (2/2)-Tetradec-1-en-1-ol 1678 - 0.5±0.04 95 1.3-Methyltetradecanal 1681 0.40±0.11 - 96 (Z)-Heptadeca-8-ene 1703 5.85±0.26 2.45±0.01 97 Heptadecane 1736 0.29±0.01 - 96 Methyl tetradecanaet 1780 0.29±0.01 - 97 <td>83</td> <td>1-Bromododecane</td> <td>1552</td> <td>_</td> <td>0.70±0.03</td>	83	1-Bromododecane	1552	_	0.70±0.03
85 Teradecan-2-one 1569 0.30t0.15 1.1810.04 86 Hexadec-1-ene 1579 1.29t0.17 1.3910.03 87 Tridecanenitrile 1592 - 0.29t0.05 88 Hexadecane 1600 0.45t0.02 1.07t0.07 90 Tetradecane 1603 1.58t0.06 4.06t0.01 90 Tetradecanel 1603 1.58t0.06 4.06t0.01 91 3-[1-Hydroxy-2-(methylanino)ethylphenol (Phenylephrine) 1660 0.110.02 0.55t0.07 92 1-(4-isopropylphenyl)-2-methylpropyl acetate 1667 - 0.45t0.15 93 (2)-Tetradec-1-en-1-ol 1679 - 0.51t0.04 94 Tetradecaneltrile 1679 - 0.51t0.04 95 13-Methyltetradecane 1687 0.91t0.06 1.08t0.03 97 Heptadecane 1703 5.85t0.26 2.45t0.01 98 Pentadecanel 171 0.63t0.01 1.08t0.06 99 Methyl Hethylehydracane 1766	84	(6E)-3,7,11-Trimethyldodeca-1,6,10-trien-3-ol (Nerolidol)	1564	0.13±0.02	0.31±0.02
86 Hexadec-1-ene 1579 1.29±0.17 1.39±0.03 87 Tridecanenitrile 1592 - 0.29±0.05 88 Hexadecane 1600 0.45±0.02 1.07±0.07 99 0.12±0.17±tradec-9-en-1-al 1603 1.5±0.06 4.06±0.01 91 3-[1-Hydroxy-2-(methylamino)ethyl]phenol (Phenylephrine) 1660 0.11±0.02 0.5±0.07 92 1.(4-Isopryphenyl)-2-methylproyal aceatae 1678 - 0.45±0.12 93 (2)-Tetradec-11-en-1.01 1678 - 0.5±0.07 94 Tetradecanenitrile 1679 - 0.5±0.02 95 1.3-Methyltetradecanal 1681 0.0410.01 - 96 (2)-Heptadec3-ene 1687 0.910.00 - 97 Heptadecanal 1711 0.63±0.01 - 108 Pentadecanal 1711 0.63±0.03 - 109 Methyl tetradecanoate 1758 0.73±0.04 0.53±0.01 101 4.Methylheptadecane 1760 0.53±0.04 1.53±0.03 102 Methyl 9-methyltetradecanoate	85	Tetradecan-2-one	1569	0.30±0.15	1.18±0.04
87 Tridecanenitrile 1592 - 0.2940.05 88 Hexadecane 1600 0.458.002 1.074.07 89 (Z)-Tetradec-9-en-1-al 1603 1.584.006 4.064.001 90 Tetradecanal 1603 0.114.002 0.554.007 91 3-[1-Hydroxy-2-(methylamino)ethyl]phenol (Phenylephrine) 1660 0.114.002 0.554.007 92 1-(4-Isopropylphenyl)-2-methylpropyl acetate 1667 - 0.454.015 93 (Z)-Tetradec-11-en-1-ol 1678 - 0.511.004 95 13-Methyltetradecanal 1681 0.404.011 - 96 (Z)-Hetptadec-3-ene 1687 0.914.006 - 97 Hetptadecanal 1711 0.6340.10 1.084.006 98 Pentadecanal 1712 0.294.001 - 100 A-Methylheptadecane 1758 0.734.004 1.534.003 102 Methyl 12-methyltetradecanoate 1790 - 0.424.011 103 Ottadec-1-ene 1790 - 0.354.004 - 104 Pentadeca	86	Hexadec-1-ene	1579	1.29±0.17	1.39±0.03
88 Hexadecane 1600 0.45±0.02 1.07±0.07 89 (2)-Tetradec-9-en-1-al 1603 1.58±0.06 4.06±0.01 90 Tetradecanal 1614 3.17±0.52 2.68±0.06 91 3-[1-Hydroxy-2-(methylamio)Phylephyl acetate 1660 0.11±0.02 0.55±0.07 92 1-(4-isopropylphenyl)-2-methylpropyl acetate 1667 - 0.45±0.15 93 (2)-Tetradec-11-en-1-0l 1678 - 0.5±0.04 95 13-Methyltetradecanal 1681 0.40±0.11 - 96 (2)-Heptadeca-3-ene 1681 0.40±0.11 - - 97 Heptadecanal 1703 5.85±0.26 2.45±0.01 1.08±0.06 99 Methyl tetradecanolate (Methyl myristate) 1726 0.29±0.01 - 100 8-Methylheptadecane 1780 0.63±0.04 1.53±0.04 1.53±0.04 101 4-Methylheptadecane 1790 - 1.24±0.11 103 Octadec-1-ene 1790 - 0.25±0.01 104 Pentadecanale (Diphenyl glycol) 1811 - 0	87	Tridecanenitrile	1592	_	0.29±0.05
89 (ζ)-Tetradec-9-en-1-al 1603 1.58±0.06 4.06±0.01 90 Tetradecanal 1614 3.17±0.52 2.68±0.06 91 3-{1-Hydroxy-2-(methylamino)[ethyl]phenol (Phenylephrine) 1660 0.11±0.02 0.55±0.07 92 1-{(4-Isopropylphenyl)-zetthyloropyla catetate 1667 - 0.45±0.15 93 (Z)-Tetradec-11-en-1-ol 1678 - 0.51±0.04 95 1.3-Methyltetradecanal 1679 - 0.51±0.04 96 (Z)-Heptadec-3-ene 1687 0.91±0.06 - 97 Heptadecane 1703 5.85±0.26 2.45±0.01 98 Pentadecanal 1711 0.63±0.10 1.08±0.06 99 Methyl tetradecanoate (Methyl myristate) 1758 0.73±0.04 0.8±0.05 101 4-Methylheptadecane 1760 0.53±0.04 1.53±0.03 - 102 Methyl 12-methyltetradecanoate 1790 - 0.3±0.01 103 Octadec-1-ene 1790 - 0.3±0.01 - 104 Pentadecanal 1792 - - 0.3±	88	Hexadecane	1600	0.45±0.02	1.07±0.07
90 Tetradecanal 1614 3.17±0.52 2.68±0.66 91 3-[1-Hydroxy-2-(methylamino)ethyllphenol (Phenylephrine) 1660 0.11±0.02 0.55±0.07 92 1-(4-Isopropylphenyl)-2-methylpropyl acetate 1667 - 0.45±0.15 93 (Z)-Tetradec-11-en-1-ol 1678 - 0.89±0.12 94 Tetradecanenitrile 1679 - 0.51±0.04 95 13-Methyltetradecanal 1681 0.40±0.11 - 96 (Z)-Heptadec-3-ene 1687 0.91±0.06 - 97 Heptadecanal 1711 0.63±0.10 1.08±0.06 99 Methyl tetradecanoate (Methyl myristate) 1726 0.29±0.01 - 100 8-Methylheptadecane 1760 0.53±0.04 1.53±0.03 101 4-Methylheptadecanoate 1786 0.68±0.03 - 103 Octadec1-ene 1790 - 0.3±0.05 104 Pentadecannel (Phytane) 1804 0.14±0.01 0.3±0.05 105 Methyl P-methyl	89	(Z)-Tetradec-9-en-1-al	1603	1.58±0.06	4.06±0.01
91 3-[1-Hydroxy-2-(methylamino)ethyllphenol (Phenylephrine) 1660 0.11±0.02 0.55±0.07 92 1-(4-Isopropylphenyl)-2-methylpropyl acetate 1667 - 0.45±0.15 93 (2)-Tetradec-11-en1-ol 1678 - 0.51±0.04 95 13-Methyltetradecanal 1681 0.40±0.11 - 96 (2)-Heptadec-3-ene 1687 0.91±0.06 - 97 Heptadecanal 1711 0.63±0.10 1.08±0.06 98 Pentadecanal 1711 0.63±0.10 - 99 Methyl tetradecanoate (Methyl myristate) 1726 0.29±0.01 - 100 8-Methylheptadecane 1758 0.73±0.04 1.53±0.03 101 4-Methylheptadecane 1760 0.53±0.04 1.53±0.03 102 Methyl 1-methyltetradecanoate 1760 0.53±0.04 - 103 Octadec-1-ene 1790 - - - 104 Pentadecanel (Phytane) 1804 0.14±0.05 - - 105 Methyl 9-methylteradecanae (Phytane) 1809 - 0.32±0.05 <	90	Tetradecanal	1614	3.17±0.52	2.68±0.06
92 1-(4-isopropylphenyl)2-methylpropyl acetate 1667 - 0.45±0.15 93 (Z)-Tetradec-11-en-1-ol 1678 - 3.89±0.12 94 Tetradecanentrile 1679 - 0.51±0.04 95 13-Methyltetradecanal 1681 0.40±0.11 - 96 (2)-Heptadec-3-ene 1687 0.91±0.06 - 97 Heptadecana 1711 0.63±0.10 1.08±0.06 98 Pentadecanal 1711 0.63±0.10 1.08±0.06 99 Methyl tetradecanate (Methyl myristate) 1726 0.29±0.01 - 100 &-Methylheptadecane 1760 0.53±0.04 1.53±0.03 102 Methyl 12-methyltetradecanoate 1760 0.68±0.03 - 103 Octadec1-ene 1790 - 0.35±0.04 1.53±0.03 104 Pentadecanenitrile 1792 - 1.24±0.11 105 Methyl 9-methyltetradecanoate 1793 - - 106 Octadecane 1804	91	3-[1-Hydroxy-2-(methylamino)ethyl]phenol (Phenylephrine)	1660	0.11±0.02	0.55±0.07
93 (Z)-Tetradec-11-en-1-ol 1678 - 3.89±0.12 94 Tetradecanenitrile 1679 - 0.51±0.04 95 13-Methyltetradecanal 1681 0.40±0.11 - 96 (Z)-Heptadec-3-ene 1687 0.91±0.06 - 97 Heptadecane 1687 0.91±0.06 1.08±0.06 98 Pentadecanal 1711 0.63±0.10 1.08±0.06 99 Methyl tetradecanoate (Methyl myristate) 1726 0.29±0.01 - 100 8-Methylheptadecane 1758 0.73±0.04 0.88±0.05 101 4-Methylheptadecane 1758 0.73±0.04 0.88±0.05 102 Methyl 12-methyltetradecanoate 1766 0.68±0.03 - 103 Octadec-1-ene 1790 - 0.35±0.01 - 104 Pentadecanenitrile 1793 - - - 105 Methyl 9-methyltetradecanal 1829 - 0.32±0.05 108 2.Phenoxyethoxybenzene (Diphenyl glycol)	92	1-(4-Isopropylphenyl)-2-methylpropyl acetate	1667	_	0.45±0.15
94 Tetradecanenitrile 1679 - 0.51±0.04 95 13-Methyltetradecanal 1681 0.40±0.11 - 96 (Z)-Heptadeca-3-ene 1687 0.91±0.06 - 97 Heptadecanal 1703 5.85±0.26 2.45±0.01 98 Pentadecanal 1711 0.63±0.10 1.08±0.06 99 Methyl tetradecanoate (Methyl myristate) 1726 0.29±0.01 - 100 8-Methylheptadecane 1760 0.53±0.04 0.88±0.03 - 101 4-Methylheptadecane 1760 0.53±0.04 0.88±0.03 - 102 Methyl 12-methyltetradecanoate 1786 0.68±0.03 - 0.35±0.04 1.53±0.03 102 Methyl 9-methyltetradecanoate 1790 - 0.35±0.04 1.53±0.03 105 Methyl 9-methyltetradecanoate 1793 - - 106 Octadecane 1809 - 0.31±0.07 107 2,6,10,14-Tetramethylkeadecane(Phytane) 1822 - <	93	(Z)-Tetradec-11-en-1-ol	1678	_	3.89±0.12
95 13-Methyltetradecanal 1681 0.40±0.11 - 96 (Z)-Heptadec-3-ene 1687 0.91±0.06 - 97 Heptadecanal 1703 5.85±0.26 2.45±0.01 98 Pentadecanal 1711 0.63±0.01 - 99 Methyl tetradecanoate (Methyl myristate) 1726 0.29±0.01 - 100 8-Methylheptadecane 1758 0.73±0.04 0.88±0.05 101 4.4Methylheptadecane 1760 0.53±0.04 1.53±0.03 102 Methyl 12-methyltetradecanoate 1786 0.68±0.03 - 103 Octadec-1-ene 1790 - 0.35±0.17 104 Pentadecanenitrile 1792 - - 105 Methyl 9-methyltetradecanoate 1786 0.42±0.05 - 106 Octadecane 1804 0.14±0.05 - - 107 2,6,10,14-Tetramethylhexadecane (Phytane) 1801 - 0.21±0.07 108 2.7,11-Trimethyldedaca-2,6,10-trienyl acetate (Farnesyl acetane) 1844 - 0.21±0.07 110 <	94	Tetradecanenitrile	1679	_	0.51±0.04
96 (Z)-Heptadeca-ene 1687 0.91±0.06 - 97 Heptadecane 1703 5.85±0.26 2.45±0.01 98 Pentadecanal 1711 0.63±0.10 1.08±0.06 99 Methyl tetradecanoate (Methyl myristate) 1726 0.29±0.01 - 100 8-Methylheptadecane 1758 0.73±0.04 0.88±0.05 101 4-Methylheptadecane 1760 0.53±0.04 1.83±0.03 102 Methyl 12-methyltetradecanoate 1786 0.68±0.03 - 103 Octadec-1-ene 1790 - 0.35±0.17 104 Pentadecanenitrile 1792 - 1.24±0.11 105 Methyl 9-methyltetradecanoate 1793 - - 106 Octadecane 1804 0.14±0.05 - 107 2,6,10,14-Tetramethylhexadecan (Phytane) 1809 - 0.32±0.05 108 2.Phenoxyethoxybenzene (Diphenyl glycol) 1811 - 0.21±0.07 109 Hexadecan-1.0 1822	95	13-Methyltetradecanal	1681	0.40±0.11	-
97 Heptadecane 1703 5.85±0.26 2.45±0.01 98 Pentadecanal 1711 0.63±0.10 1.08±0.06 99 Methyl tetradecanoate (Methyl myristate) 1726 0.29±0.01 - 100 8-Methylheptadecane 1758 0.73±0.04 0.88±0.05 101 4-Methylheptadecane 1760 0.53±0.04 1.53±0.03 102 Methyl 12-methyltetradecanoate 1786 0.68±0.03 - 103 Octadec-1-ene 1790 - 0.35±0.17 104 Pentadecanenitrile 1793 - - 105 Methyl 9-methyltetradecanoate 1793 - - 106 Octadecane 1809 - 0.32±0.05 108 2-Phenoxyethoxybenzene (Diphenyl glycol) 1811 - 0.21±0.07 109 Hexadecanal 1822 - 0.31±0.07 110 3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate) 1844 - 0.27±0.27 111 6,10,14-Trimethylpentadecan-2-one (96	(Z)-Heptadec-3-ene	1687	0.91±0.06	_
98 Pentadecanal 1711 0.63±0.10 1.08±0.06 99 Methyl tetradecanoate (Methyl myristate) 1726 0.29±0.01 - 100 &-Methylheptadecane 1758 0.73±0.04 0.88±0.05 101 4-Methylheptadecane 1760 0.53±0.04 1.53±0.03 102 Methyl 12-methyltetradecanoate 1786 0.68±0.03 - 103 Octadec-1-ene 1790 - 0.35±0.17 104 Pentadecanenitrile 1792 - 1.24±0.11 105 Methyl 9-methyltetradecanoate 1793 - - 106 Octadecane 1804 0.14±0.05 - 107 2,6,10,14-Tetramethylhexadecane (Phytane) 1809 - 0.32±0.07 108 2-Phenoxyethoxybenzene (Diphenyl glycol) 1811 - 0.21±0.07 109 Hexadecanal 1822 - 0.31±0.07 110 3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate) 1844 - 0.27±0.27 111 6,10	97	Heptadecane	1703	5.85±0.26	2.45±0.01
99 Methyl tetradecanoate (Methyl myristate) 1726 0.29±0.01 - 100 8-Methylheptadecane 1758 0.73±0.04 0.88±0.05 101 4-Methylheptadecane 1760 0.53±0.04 1.53±0.03 102 Methyl 12-methyltetradecanoate 1786 0.68±0.03 - 103 Octadec-1-ene 1790 - 0.35±0.17 104 Pentadecanenitrile 1792 - 1.24±0.11 105 Methyl 9-methyltetradecanoate 1793 - - 106 Octadecane 1804 0.14±0.05 - 107 2,6,10,14-Tetramethylhexadecane (Phytane) 1809 - 0.32±0.05 108 2-Phenoxyethoxybenzene (Diphenyl glycol) 1811 - 0.21±0.07 109 Hexadecanal 1822 - 0.31±0.07 110 6,10,14-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate) 1844 - 0.27±0.27 111 6,10,14-Trimethylgentadecan-2-one (Hexahydrofarnesyl acetane) 1846 0.14±0.01 0.47±0.19 <	98	Pentadecanal	1711	0.63±0.10	1.08±0.06
100 8-Methylheptadecane 1758 0.73±0.04 0.88±0.05 101 4-Methylheptadecane 1760 0.53±0.04 1.53±0.03 102 Methyl 12-methyltetradecanoate 1786 0.68±0.03 - 103 Octadec-1-ene 1790 - 0.35±0.17 104 Pentadecanenitrile 1792 - 1.24±0.11 105 Methyl 9-methyltetradecanoate 1793 - - 106 Octadecane 1804 0.14±0.05 - 107 2,6,10,14-Tetramethylhexadecane (Phytane) 1809 - 0.32±0.05 108 2-Phenoxyethoxybenzene (Diphenyl glycol) 1811 - 0.21±0.07 109 Hexadecanal 1822 - 0.31±0.07 110 3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate) 1844 - 0.27±0.27 111 6,10,14-Trimethyldoeta-2,6,10-trienyl acetate (Farnesyl acetate) 1846 0.14±0.01 0.45±0.27 112 (92)-Hexadec-1,9-diene 1863 - 0.47±0.19 111 113 (2)-Hexadec-1,enal 1871 - 0.	99	Methyl tetradecanoate (Methyl myristate)	1726	0.29±0.01	_
101 4-Methylheptadecane 1760 0.53±0.04 1.53±0.03 102 Methyl 12-methyltetradecanoate 1786 0.68±0.03 - 103 Octadec-1-ene 1790 - 0.35±0.17 104 Pentadecanenitrile 1792 - 1.24±0.11 105 Methyl 9-methyltetradecanoate 1793 - - 106 Octadecane 1804 0.14±0.05 - 107 2,6,10,14-Tetramethylhexadecane (Phytane) 1809 - 0.32±0.05 108 2-Phenoxyethoxybenzene (Diphenyl glycol) 1811 - 0.21±0.07 109 Hexadecanal 1822 - 0.31±0.07 110 3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate) 1844 - 0.27±0.27 111 6,10,14-Trimethylpentadecan-2-one (Hexahydrofarnesyl acetane) 1846 0.14±0.01 0.45±0.27 112 (92)-Hexadec-11-enal 1863 - 0.15±0.15 113 (Z)-Hexadec-11-enal 1871 - 0.15±0.15 114 bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate) 1883 0.	100	8-Methylheptadecane	1758	0.73±0.04	0.88±0.05
102 Methyl 12-methyltetradecanoate 1786 0.68±0.03 - 103 Octadec-1-ene 1790 - 0.35±0.17 104 Pentadecanenitrile 1792 - 1.24±0.11 105 Methyl 9-methyltetradecanoate 1793 - - 106 Octadecane 1804 0.14±0.05 - 107 2,6,10,14-Tetramethylhexadecane (Phytane) 1809 - 0.32±0.05 108 2-Phenoxyethoxybenzene (Diphenyl glycol) 1811 - 0.21±0.07 109 Hexadecanal 1822 - 0.31±0.07 110 3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate) 1844 - 0.27±0.27 111 6,10,14-Trimethylpentadecan-2-one (Hexahydrofarnesyl acetane) 1846 0.14±0.01 0.45±0.27 112 (92)-Hexadeca-1,9-diene 1863 - 0.15±0.15 113 (Z)-Hexadec-11-enal 1871 - 0.15±0.15 114 bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate) 1883 0.37±0.08 2.04±0.52 115 Hexadecan-1-ol 1883 0.37	101	4-Methylheptadecane	1760	0.53±0.04	1.53±0.03
103 Octadec-1-ene 1790 - 0.35±0.17 104 Pentadecanenitrile 1792 - 1.24±0.11 105 Methyl 9-methyltetradecanoate 1793 - - 106 Octadecane 1804 0.14±0.05 - 107 2,6,10,14-Tetramethylhexadecane (Phytane) 1809 - 0.32±0.05 108 2-Phenoxyethoxybenzene (Diphenyl glycol) 1811 - 0.21±0.07 109 Hexadecanal 1822 - 0.31±0.07 110 3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate) 1844 - 0.27±0.27 111 6,10,14-Trimethylpentadecan-2-one (Hexahydrofarnesyl acetane) 1846 0.14±0.01 0.45±0.27 112 (92)-Hexadeca-1,9-diene 1863 - 0.47±0.19 113 (Z)-Hexadec-11-enal 1871 - 0.15±0.15 114 bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate) 1823 0.37±0.08 2.04±0.52 115 Hexadecan-1-ol 1883 0.37±0.08 2.04±0.52	102	Methyl 12-methyltetradecanoate	1786	0.68±0.03	_
104 Pentadecanenitrile 1792 - 1.24±0.11 105 Methyl 9-methyltetradecanoate 1793 - - 106 Octadecane 1804 0.14±0.05 - 107 2,6,10,14-Tetramethylhexadecane (Phytane) 1809 - 0.32±0.05 108 2-Phenoxyethoxybenzene (Diphenyl glycol) 1811 - 0.21±0.07 109 Hexadecanal 1822 - 0.31±0.07 110 3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate) 1844 - 0.27±0.27 111 6,10,14-Trimethylpentadecan-2-one (Hexahydrofarnesyl acetane) 1846 0.14±0.01 0.45±0.27 112 (92)-Hexadeca-1,9-diene 1863 - 0.47±0.19 113 (Z)-Hexadec-11-enal 1871 - 0.15±0.15 114 bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate) 1872 8.44±1.12 1.80±0.57 115 Hexadecan-1-ol 1883 0.37±0.08 2.04±0.52 115 Hexadecan-1-ol 1883 0.37±0.08 2.04±0.52	103	Octadec-1-ene	1790	-	0.35±0.17
105 Methyl 9-methyltetradecanoate 1793 - - 106 Octadecane 1804 0.14±0.05 - 107 2,6,10,14-Tetramethylhexadecane (Phytane) 1809 - 0.32±0.05 108 2-Phenoxyethoxybenzene (Diphenyl glycol) 1811 - 0.21±0.07 109 Hexadecanal 1822 - 0.31±0.07 110 3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate) 1844 - 0.27±0.27 111 6,10,14-Trimethylpentadecan-2-one (Hexahydrofarnesyl acetone) 1863 - 0.47±0.19 112 (92)-Hexadeca-1,9-diene 1863 - 0.15±0.15 113 (Z)-Hexadec-11-enal 1871 - 0.15±0.15 114 bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate) 1872 8.44±1.12 1.80±0.57 115 Hexadecan-1-ol 1883 0.37±0.08 2.04±0.52	104	Pentadecanenitrile	1792	-	1.24±0.11
106 Octadecane 1804 0.14±0.05 - 107 2,6,10,14-Tetramethylhexadecane (Phytane) 1809 - 0.32±0.05 108 2-Phenoxyethoxybenzene (Diphenyl glycol) 1811 - 0.21±0.07 109 Hexadecanal 1822 - 0.31±0.07 110 3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate) 1844 - 0.27±0.27 111 6,10,14-Trimethylpentadecan-2-one (Hexahydrofarnesyl acetone) 1846 0.14±0.01 0.45±0.27 112 (92)-Hexadeca-1,9-diene 1863 - 0.47±0.19 113 (Z)-Hexadec-11-enal 1871 - 0.15±0.15 114 bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate) 1872 8.44±1.12 1.80±0.57 115 Hexadecan-1-ol 1883 0.37±0.08 2.04±0.52 * SD is the standard deviation of sample triplicate: RI – retention index. - -	105	Methyl 9-methyltetradecanoate	1793	-	_
107 2,6,10,14-Tetramethylhexadecane (Phytane) 1809 - 0.32±0.05 108 2-Phenoxyethoxybenzene (Diphenyl glycol) 1811 - 0.21±0.07 109 Hexadecanal 1822 - 0.31±0.07 110 3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate) 1844 - 0.27±0.27 111 6,10,14-Trimethylpentadecan-2-one (Hexahydrofarnesyl acetone) 1846 0.14±0.01 0.45±0.27 112 (92)-Hexadeca-1,9-diene 1863 - 0.47±0.19 113 (Z)-Hexadec-11-enal 1871 - 0.15±0.15 114 bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate) 1872 8.44±1.12 1.80±0.57 115 Hexadecan-1-ol 1883 0.37±0.08 2.04±0.52 * SD is the standard deviation of sample triplicate: RI – retention index. * * * * *	106	Octadecane	1804	0.14±0.05	-
108 2-Phenoxyethoxybenzene (Diphenyl glycol) 1811 - 0.21±0.07 109 Hexadecanal 1822 - 0.31±0.07 110 3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate) 1844 - 0.27±0.27 111 6,10,14-Trimethylpentadecan-2-one (Hexahydrofarnesyl acetane) 1846 0.14±0.01 0.45±0.27 112 (92)-Hexadeca-1,9-diene 1863 - 0.47±0.19 113 (Z)-Hexadec-11-enal 1871 - 0.15±0.15 114 bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate) 1872 8.44±1.12 1.80±0.57 115 Hexadecan-1-ol 1883 0.37±0.08 2.04±0.52 * SD is the standard deviation of sample triplicate: RI – retention index.	107	2,6,10,14-Tetramethylhexadecane (Phytane)	1809	_	0.32±0.05
109 Hexadecanal 1822 - 0.31±0.07 110 3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate) 1844 - 0.27±0.27 111 6,10,14-Trimethylpentadecan-2-one (Hexahydrofarnesyl acetone) 1846 0.14±0.01 0.45±0.27 112 (92)-Hexadeca-1,9-diene 1863 - 0.47±0.19 113 (Z)-Hexadec-11-enal 1871 - 0.15±0.15 114 bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate) 1872 8.44±1.12 1.80±0.57 115 Hexadecan-1-ol 1883 0.37±0.08 2.04±0.52 * SD is the standard deviation of sample triplicate: RI – retention index.	108	2-Phenoxyethoxybenzene (Diphenyl glycol)	1811	-	0.21±0.07
110 3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate) 1844 - 0.27±0.27 111 6,10,14-Trimethylpentadecan-2-one (Hexahydrofarnesyl acetone) 1846 0.14±0.01 0.45±0.27 112 (92)-Hexadeca-1,9-diene 1863 - 0.47±0.19 113 (2)-Hexadec-11-enal 1871 - 0.15±0.15 114 bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate) 1872 8.44±1.12 1.80±0.57 115 Hexadecan-1-ol 1883 0.37±0.08 2.04±0.52 * SD is the standard deviation of sample triplicate: RI – retention index.	109	Hexadecanal	1822	-	0.31±0.07
111 6,10,14-Trimethylpentadecan-2-one (Hexahydrofarnesyl acetone) 1846 0.14±0.01 0.45±0.27 112 (92)-Hexadeca-1,9-diene 1863 - 0.47±0.19 113 (2)-Hexadec-11-enal 1871 - 0.15±0.15 114 bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate) 1872 8.44±1.12 1.80±0.57 115 Hexadecan-1-ol 1883 0.37±0.08 2.04±0.52 * SD is the standard deviation of sample triplicate: RI – retention index. - -	110	3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (Farnesyl acetate)	1844	-	0.27±0.27
112 (92)-Hexadeca-1,9-diene 1863 - 0.47±0.19 113 (2)-Hexadec-11-enal 1871 - 0.15±0.15 114 bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate) 1872 8.44±1.12 1.80±0.57 115 Hexadecan-1-ol 1883 0.37±0.08 2.04±0.52 * SD is the standard deviation of sample triplicate: RI – retention index.	111	6,10,14-Trimethylpentadecan-2-one (Hexahydrofarnesyl acetone)	1846	0.14±0.01	0.45±0.27
113 (Z)-Hexadec-11-enal 1871 - 0.15±0.15 114 bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate) 1872 8.44±1.12 1.80±0.57 115 Hexadecan-1-ol 1883 0.37±0.08 2.04±0.52 * SD is the standard deviation of sample triplicate: RI – retention index. - - -	112	(9Z)-Hexadeca-1,9-diene	1863	_	0.47±0.19
114 bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate) 1872 8.44±1.12 1.80±0.57 115 Hexadecan-1-ol 1883 0.37±0.08 2.04±0.52 * SD is the standard deviation of sample triplicate: RI – retention index. * *	113	(Z)-Hexadec-11-enal	1871	_	0.15±0.15
115 Hexadecan-1-ol 1883 0.37±0.08 2.04±0.52 * SD is the standard deviation of sample triplicate: RI – retention index.	114	bis(2-Methylpropyl)benzene-1,2-dicarboxylate (Diisobutyl phthalate)	1872	8.44±1.12	1.80±0.57
* SD is the standard deviation of sample triplicate: RI – retention index.	115	Hexadecan-1-ol	1883	0.37±0.08	2.04±0.52
	* SD is the	standard deviation of sample triplicate. RI – retention index			

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No.	Compound	RI	Area (%) ± SD*	
			V	VI
116	Nonadec-1-ene	1895	0.41±0.01	0.35±0.17
117	Methyl (Z)-hexadec-7-enoate	1899	3.77±0.16	-
118	(5E,9E)-6,10,14-Trimethylpentadeca-5,9,13-trien-2-one (Farnesyl acetone)	1919	0.17±0.03	0.31±0.10
119	Methyl hexadecanoate (Methyl palmitate)	1926	0.63±0.05	-
120	1-(Pentyloxy)tetradecane	1971	-	0.79±0.18
121	Methyl 14-methylhexadecanoate	1975	1.22±0.10	-
122	Ethyl (E)-hexadec-9-enoate	1979	3.66±0.26	-
123	lcos-1-ene	1992	-	0.15±0.09
124	Icosane	2000	-	0.12±0.12
125	(Z)-Methyl heptadec-10-enoate	2015	0.21±0.01	-
126	(6E,10E)-3,7,11,15-Tetramethylhexadeca-1,6,10,14-tetraen-3-ol	2032	0.21±0.03	0.64±0.21
127	3,8-Dimethyl-5-[6-methylhept-5-en-2-yl]-(1,3a,4,5,6,8a)-hexahydroazulen-4-ol (Isopachydictyol A)	2130	0.73±0.04	-

* SD is the standard deviation of sample triplicate; RI - retention index.



Figure 3. The volatile organic compounds (VOCs) of *P. ficiformis* obtained by hydrodistillation (HD), analysed by gas chromatography–mass spectrometry (GC-MS) and sorted by structural groups. HD-FrPF – hydrodistillate of fresh *P. ficiformis*; HD-DrPF – hydrodistillate of air-dried *P. ficiformis*.



Figure 4. The most abundant compounds of *P. ficiformis* samples obtained by hydrodistillation (HD) and analysed by gas chromatography–mass spectrometry (GC-MS). HD-FrPF – hydrodistillate of fresh *P. ficiformis*; HD-DrPF – hydrodistillate of air-dried *P. ficiformis*.



CONCLUSION

Since there is no data available on P. ficiformis VOCs in the literature and only scarce data regarding polyacetylenes, sterols and phospholipids are present, this paper offers a detailed research on P. ficiformis VOCs profile for the first time. Aliphatic compounds were dominant in both FrPH and DrPF samples extracted by HS-SPME and in HD. Heptadecane was the most abundant hydrocarbon in the headspace samples with higher abundance in HS-DrPH and the second most abundant aliphatic compound in HD-FrPH, but with much lower abundance than in the headspace of the samples extracted by HS-SPME. The second most dominant group of compounds were benzene derivatives in both samples. In the headspace of the samples, benzene derivatives with the highest abundance were benzaldehyde and benzyl alcohol and in HD diisobutyl phthalate, 1,4xylene and benzaldehyde. The great difference between fresh and air-dried samples was noticed in terms of fatty acids and derivatives abundance. Two hexadecanoic acid esters, methyl (Z)-hexadec-7-enoate and ethyl (E)-hexadec-9-enoate, were identified in HD-FrPF in higher abundance but were not detected in HD-DrPF. The compounds containing sulphur, especially dimethyl trisulphide, were mostly detected in HD-DrPF, probably causing an unpleasant smell. The compounds containing nitrogen were present in a higher portion in the samples after airdrying in both types of isolation, particularly N,Ndimethylmethanamine in the headspace. The second most abundant compound in HD-DrPF was 1H-indole. Few terpenes, C13-norisoprenoides and chlorophyll derivatives were detected mostly in HD-DrPF. By choosing different methods of isolation of P. ficiformis VOCs their more complete profile was obtained for the first time.

List Of Abbrevations

VOCs	volatile organic compounds
WoRMS	Word Register of Marine Species
GC-MS	gas chromatography-mass spectrometry
HS-SPME	headspace solid-phase microextraction
HD	hydrodistillation
FrPF	fresh P. ficiformis
DrPF	dry P. ficiformis
DVB/CAR/PDM	S divinylbenzene/carboxene/polydimethylsiloxane
PDMS/DVB	polydimethylsiloxane/divinylbenzene
f1	DVB/CAR/PDMS fibre
f2	PDMS/DVB fibre
HS-FrPF	headspace composition of fresh P. ficiformis
HS-DrPF	headspace composition of dry P. ficiformis
HD-FrPF	hydrodistillate of fresh P. ficiformis
HD-DrPF	hydrodistillate of dry P. ficiformis

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