ADDITIONAL MATERIALS

to «**Composition of the Low Molecular Weight Metabolome of *Potamogeton perfoliatus* L. (Potamogetonaceae) as an Indicator of the Transformation of the Ecological State of the Littoral Zone»**

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Table S1*.* Component composition of the essential oil of *P. perfoliatus* from diverse habitats in Lake Ladoga (RI is the retention index; % is the percentage of the substance from the sum of all substances of the essential oil; C is the absolute content of substances, µg/g of dry plant weight)

| **Component** | **Formula** | **RI** | **Volkhovskaja Bay** | **Impilakhti** | **Lekhmolakhti** | **Voronovo** | **Mantinsaari** | **Svirskaja Bay** |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **%** | **C** | **%** | **C** | **%** | **C** | **%** | **C** | **%** | **C** | **%** | **C** |
| ***hexan-3-one*** | **C6H12O** | ***791*** | ***3.04*** | ***0.98*** |  |  |  |  | ***0.65*** | ***0.56*** | ***0.17*** | ***0.46*** | ***1.08*** | ***0.43*** |
| ***hexan-2-one*** | **C6H12O** | ***794*** | ***4.42*** | ***1.42*** |  |  |  |  | ***1.64*** | ***1.41*** | ***0.47*** | ***1.27*** | ***2.86*** | ***1.14*** |
| hexan-3-ol | C6H14O | 798 | 0.42 | 0.13 |  |  |  |  | 0.40 | 0.34 | 0.14 | 0.39 |  |  |
| ***hexanal*** | **C6H12O** | ***799*** | ***3.35*** | ***1.08*** | ***2.95*** | ***0.64*** |  |  | ***1.23*** | ***1.06*** | ***0.15*** | ***0.41*** | ***1.53*** | ***0.61*** |
| ***hexan-2-ol*** | **C6H14O** | ***802*** | ***1.04*** | ***0.33*** |  |  |  |  | ***0.28*** | ***0.25*** | ***0.13*** | ***0.35*** | ***0.33*** | ***0.13*** |
| furan-2-carbaldehyde | C5H4O2 | 824 | 0.08 | 0.03 |  |  |  |  |  |  | 0.08 | 0.22 |  |  |
| ***(E)-hex-2-en-1-ol*** | **C6H12O** | ***838*** | ***1.62*** | ***0.52*** |  |  |  |  | ***0.79*** | ***0.68*** | ***0.50*** | ***1.35*** | ***1.93*** | ***0.77*** |
| ***(E)-hex-2-enal*** | **C6H10O** | ***843*** | ***10.86*** | ***3.49*** | ***10.05*** | ***2.17*** | ***1.72*** | ***2.03*** | ***2.61*** | ***2.25*** | ***2.10*** | ***5.64*** | ***10.83*** | ***4.31*** |
| ethylbenzene | C8H10 | 858 |  |  |  |  |  |  |  |  |  |  | 0.35 | 0.14 |
| hexan-1-ol | C6H14O | 869 |  |  |  |  |  |  | 0.10 | 0.09 | 0.06 | 0.16 | 0.03 | 0.01 |
| hexane-2,4-dione | C6H10O2 | 874 |  |  |  |  |  |  | 0.04 | 0.03 | 0.02 | 0.05 | 0.10 | 0.04 |
| 1,3-xylene | C8H10 | 883 | 0.69 | 0.22 |  |  |  |  | 0.13 | 0.11 | 0.05 | 0.14 | 0.23 | 0.09 |
| 1,4-xylene  | C8H10 | 889 | 0.40 | 0.13 | 0.22 | 0.05 |  |  | 0.13 | 0.11 | 0.16 | 0.44 |  |  |
| heptan-2-one  | C7H14O | 890 | 0.44 | 0.14 | 0.29 | 0.06 |  |  | 0.13 | 0.11 | 0.03 | 0.07 | 0.20 | 0.08 |
| ***1,2-xylene*** | **C8H10** | ***897*** |  |  |  |  | ***1.12*** | ***1.33*** |  |  |  |  |  |  |
| (Z)-hept-4-enal | C7H12O | 898 | 0.65 | 0.21 |  |  |  |  | 0.14 | 0.12 | 0.05 | 0.15 | 0.08 | 0.03 |
| heptanal | C7H14O | 901 | 0.53 | 0.17 | 0.78 | 0.17 | 0.44 | 0.52 | 0.22 | 0.19 | 0.31 | 0.83 | 0.68 | 0.27 |
| (E)-hept-4-enal  | C7H12O | 903 |  |  | 0.32 | 0.07 |  |  |  |  |  |  |  |  |
| nonane  | C9H20 | 906 |  |  |  |  | 0.17 | 0.21 |  |  |  |  |  |  |
| (2E,4E)-hexa-2,4-dienal | C6H8O | 910 | 0.77 | 0.25 | 0.22 | 0.05 | 0.02 | 0.03 | 0.16 | 0.14 | 0.08 | 0.21 | 0.35 | 0.14 |
| oxolan-2-ylmethanol | C5H10O2 | 913 |  |  |  |  |  |  | 0.16 | 0.14 | 0.04 | 0.10 | 0.18 | 0.07 |
| 4-ethylphenol | C8H10O | 915 |  |  |  |  |  |  | 0.08 | 0.07 |  |  |  |  |
| cyclopenta-1,3-diene | C9H14 | 918 |  |  | 0.14 | 0.03 |  |  |  |  |  |  |  |  |
| 2,6-dimethyloctane  | C10H22 | 934 |  |  |  |  | 0.01 | 0.02 |  |  |  |  |  |  |
| 3-hepten-2-one | C7H12O | 936 |  |  |  |  |  |  |  |  |  |  | 0.15 | 0.06 |
| 6-methylhept-5-en-2-one | C8H14O | 943 |  |  |  |  | 0.02 | 0.02 | 0.32 | 0.28 |  |  |  |  |
| ***benzaldehyde*** | **C7H6O** | ***949*** | ***1.69*** | ***0.54*** | ***1.50*** | ***0.32*** | ***0.10*** | ***0.11*** | ***0.75*** | ***0.65*** | ***0.22*** | ***0.59*** | ***0.78*** | ***0.31*** |
| 1,3,5-trimethylbenzene | C9H12 | 957 |  |  |  |  | 0.02 | 0.02 | 0.05 | 0.04 | 0.03 | 0.09 | 0.08 | 0.03 |
| 2-hydroperoxyheptane | C7H16O2 | 961 |  |  |  |  |  |  | 0.07 | 0.06 |  |  | 0.05 | 0.02 |
| ***2,4-dimethylocta-2,6-diene*** | **C10H18** | ***967*** | ***1.15*** | ***0.37*** |  |  |  |  | ***0.64*** | ***0.56*** | ***0.16*** | ***0.43*** |  |  |
| 1-cyclohexylethanone | C8H14O | 967 |  |  |  |  |  |  |  |  |  |  | 0.78 | 0.31 |
| 4-methylcyclohexan-1-one | C7H12O | 969 |  |  |  |  | 0.05 | 0.06 |  |  |  |  |  |  |
| 3-aminopyrrolidine-2,5-dione | C4H6N2O2 | 976 | 0.54 | 0.17 |  |  |  |  | 0.14 | 0.12 | 0.01 | 0.04 |  |  |
| Unidentified m/z 133 [M+]. 86 (100) |  | 976 |  |  |  |  |  |  |  |  |  |  | 0.23 | 0.09 |
| oct-1-en-3-ol | C8H16O | 982 |  |  | 0.21 | 0.05 |  |  |  |  |  |  |  |  |
| 2-methyloctan-3-one | C9H18O | 984 |  |  |  |  |  |  |  |  |  |  | 0.98 | 0.39 |
| ***oct-7-en-2-one*** | **C8H14O** | ***984*** | ***1.77*** | ***0.57*** | ***2.92*** | ***0.63*** |  |  | ***0.46*** | ***0.39*** | ***0.16*** | ***0.43*** |  |  |
| 6-methylhept-5-en-2-one | C8H14O | 987 |  |  |  |  |  |  |  |  |  |  |  |  |
| (E)-oct-6-en-2-one | C8H14O | 987 |  |  |  |  | 0.28 | 0.33 |  |  |  |  |  |  |
| 1-methylbicyclo[2.2.1]heptan-2-ol | C8H14O | 987 |  |  |  |  |  |  |  |  |  |  | 0.88 | 0.35 |
| ***2-pentylfuran*** | **C9H14O** | ***987*** | ***1.29*** | ***0.42*** |  |  | ***0.22*** | ***0.26*** | ***0.45*** | ***0.39*** | ***0.21*** | ***0.56*** |  |  |
| 1-ethylcyclohexene | C8H14 | 997 |  |  |  |  |  |  |  |  |  |  | 0.30 | 0.12 |
| (4E)-3-ethylhexa-1,4-diene |  C8H14 | 998 |  |  |  |  | 0.06 | 0.07 |  |  |  |  |  |  |
| (E)-oct-3-en-2-ol | C8H16O | 998 |  |  |  |  |  |  | 0.12 | 0.10 | 0.03 | 0.08 |  |  |
| ***2-*[(*Z*)*-pent-2-enyl*]*furan*** | **C9H12O** | ***999*** | ***1.51*** | ***0.49*** |  |  |  |  | ***0.16*** | ***0.14*** | ***0.17*** | ***0.45*** | ***0.60*** | ***0.24*** |
| 2-[(E)-pent-2-enyl]furan | C9H12O | 1000 |  |  | 0.87 | 0.19 | 0.29 | 0.34 |  |  |  |  |  |  |
| **(*2E,4E*)*-hepta-2,4-dienal*** | **C7H10O** | ***1009*** | ***3.09*** | ***0.99*** | ***1.31*** | ***0.28*** | ***0.14*** | ***0.16*** | ***0.86*** | ***0.75*** | ***0.35*** | ***0.94*** | ***1.83*** | ***0.73*** |
| Unidentified m/z ? [M+], 43 (100) |  | 1014 |  |  |  |  | 0.02 | 0.02 |  |  |  |  |  |  |
| 1-methyl-4-propan-2-ylsulfanylbenzene | C10H14 | 1017 |  |  | 0.72 | 0.16 |  |  |  |  |  |  |  |  |
| **(*4R*)*-1-methyl-4-prop-1-en-2-ylcyclohexene;* [*D-Limonene*]** | **C10H16** | ***1019*** | ***1.13*** | ***0.36*** |  |  |  |  | ***0.19*** | ***0.16*** | ***0.06*** | ***0.17*** | ***0.33*** | ***0.13*** |
| 2,6-dimethyloctane | C10H22 | 1022 |  |  |  |  | 0.03 | 0.03 |  |  |  |  |  |  |
| 2,2,6-trimethylcyclohexan-1-one |  C9H16O | 1025 | 0.42 | 0.14 | 0.33 | 0.07 | 0.06 | 0.07 | 0.16 | 0.13 | 0.05 | 0.13 | 0.23 | 0.09 |
| ***2-phenylacetaldehyde*** | **C8H8O** | ***1036*** | ***1.23*** | ***0.40*** | ***1.13*** | ***0.24*** | ***0.56*** | ***0.66*** | ***0.54*** | ***0.47*** | ***0.07*** | ***0.19*** | ***0.50*** | ***0.20*** |
| 3,5-octadien-2-ol | C8H14O | 1040 |  |  |  |  |  |  |  |  |  |  | 0.10 | 0.04 |
| 4-acetyl-1-methylcyclohexene | C9H14O | 1047 |  |  |  |  |  |  |  |  |  |  | 0.05 | 0.02 |
| Unidentified m/z ? [M+], 69 (100) |  | 1047 |  |  |  |  | 0.02 | 0.03 |  |  |  |  |  |  |
| 2-methyl-5-(1-methylethyl)-1,3-cyclohexadiene | C10H16 | 1049 |  |  |  |  |  |  |  |  |  |  | 0.05 | 0.02 |
| 3,5,5-trimethylcyclohex-2-en-1-one; [Isoforon] | C9H14O | 1050 |  |  | 0.20 | 0.04 | 0.02 | 0.03 |  |  |  |  |  |  |
| 3,6,6-trimethylcyclohex-2-en-1-one | C9H14O | 1050 | 0.13 | 0.04 |  |  |  |  | 0.12 | 0.10 | 0.02 | 0.05 | 0.10 | 0.04 |
| (E)-oct-2-enal | C8H14O | 1054 | 0.14 | 0.05 | 0.33 | 0.07 | 0.06 | 0.08 | 0.12 | 0.10 | 0.03 | 0.08 | 0.20 | 0.08 |
| 4-methylbenzaldehyde | C8H8O | 1058 | 0.05 | 0.02 | 0.42 | 0.09 |  |  | 0.14 | 0.12 | 0.03 | 0.09 | 0.15 | 0.06 |
| (3E,5E)-octa-3,5-dien-2-one (isomer) | C8H12O | 1068 | 0.56 | 0.18 | 1.84 | 0.40 | 0.10 | 0.12 | 0.23 | 0.20 | 0.08 | 0.22 |  |  |
| **(*3E,5E*)*-octa-3,5-dien-2-one***  | **C8H12O** | ***1072*** | ***1.80*** | ***0.58*** |  |  | ***0.11*** | ***0.13*** | ***0.56*** | ***0.49*** | ***0.16*** | ***0.42*** | ***0.65*** | ***0.26*** |
| 2-methyl-1-(2-propan-2-ylcyclopropyl)propan-1-one | C10H18O | 1075 |  |  |  |  | 0.03 | 0.04 |  |  |  |  |  |  |
| 4,7,7-trimethylbicyclo[2.2.1]heptan-2-ol; [3-Bornanol]  | C10H18O | 1087 | 0.32 | 0.10 |  |  |  |  | 0.09 | 0.08 | 0.01 | 0.03 |  |  |
| Unidentified m/z 280 [M+]. 124 (100) |  | 1088 |  |  |  |  |  |  |  |  |  |  | 0.10 | 0.04 |
| 3,5-octadiene-2-one (isomer) | C8H12O | 1095 |  |  |  |  |  |  |  |  |  |  | 0.53 | 0.21 |
| ***2,6-dimethylcyclohexan-1-ol*** | **C8H16O** | ***1099*** | ***1.76*** | ***0.57*** | ***0.69*** | ***0.15*** | ***0.05*** | ***0.06*** | ***0.37*** | ***0.32*** | ***0.12*** | ***0.32*** | ***0.60*** | ***0.24*** |
| nonanal | C9H18O | 1100 | 0.27 | 0.09 | 0.85 | 0.18 | 0.70 | 0.82 | 0.23 | 0.20 | 0.21 | 0.55 | 0.35 | 0.14 |
| (1S,5R)-3,3,5-trimethylcyclohexan-1-ol | C9H18O | 1106 |  |  |  |  |  |  | 0.16 | 0.14 | 0.01 | 0.03 | 0.23 | 0.09 |
| ***2,6,6-trimethylcyclohex-2-ene-1,4-dione;* [*oxophoron*]** | **C9H12O2** | ***1136*** | ***1.90*** | ***0.61*** | ***0.80*** | ***0.17*** | ***0.05*** | ***0.06*** | ***0.39*** | ***0.34*** | ***0.04*** | ***0.10*** | ***0.75*** | ***0.30*** |
| Unidentified m/z ? [M+], 98 (100) |  C9H14O2 | 1139 |  |  |  |  |  |  | 0.09 | 0.07 | 0.06 | 0.16 | 0.20 | 0.08 |
| 5-methyl-2-propan-2-yl-6-oxabicyclo[3.1.0]hexane-1-carbaldehyde | C10H16O2 | 1143 |  |  |  |  | 0.03 | 0.03 |  |  |  |  |  |  |
| (2E,6Z)-nona-2,6-dienal | C9H14O | 1150 |  |  |  |  | 0.04 | 0.04 |  |  | 0.03 | 0.08 | 0.18 | 0.07 |
| 1-phenylpropan-1-one | C9H10O | 1156 |  |  |  |  |  |  |  |  |  |  | 0.08 | 0.03 |
| (E)-non-2-enal | C9H16O | 1157 |  |  |  |  | 0.07 | 0.08 |  |  |  |  |  |  |
| 4-ethylbenzaldehyde | C9H10O | 1165 |  |  |  |  |  |  |  |  |  |  | 0.13 | 0.05 |
| naphthalene | C10H8 | 1166 |  |  | 0.58 | 0.13 |  |  |  |  |  |  |  |  |
| 3-ethylbenzaldehyde | C9H10O | 1166 |  |  |  |  |  |  |  |  | 0.05 | 0.14 |  |  |
| 2,6,6-trimethylcyclohexa-1,3-diene-1-carbaldehyde; [Safranal] | C10H14O | 1189 | 0.35 | 0.11 | 0.51 | 0.11 | 0.07 | 0.08 | 0.15 | 0.13 | 0.08 | 0.22 | 0.40 | 0.16 |
| octanoic acid | C8H16O2 | 1196 |  |  |  |  | 0.02 | 0.02 |  |  |  |  |  |  |
| ***dodecane*** | **C12H26** | ***1200*** | ***1.88*** | ***0.60*** | ***0.47*** | ***0.10*** |  |  | ***0.33*** | ***0.28*** | ***0.15*** | ***0.40*** | ***0.63*** | ***0.25*** |
| 1,3-benzothiazole | C7H5NS | 1210 |  |  | 1.05 | 0.23 |  |  |  |  |  |  |  |  |
| 2,6,6-trimethylcyclohexene-1-carbaldehyde; [β-cyclocitral] | C10H16O | 1210 | 0.39 | 0.12 | 0.32 | 0.07 | 0.07 | 0.09 | 0.18 | 0.16 | 0.13 | 0.35 | 0.38 | 0.15 |
| 3,4,5-trimethylcyclohex-3-ene-1-carbaldehyde | C10H16O | 1215 |  |  |  |  | 0.05 | 0.06 |  |  |  |  |  |  |
| 2-cyclopentylcyclopentan-1-one | C10H16O | 1218 |  |  |  |  |  |  | 0.06 | 0.05 | 0.04 | 0.11 |  |  |
| Unidentified m/z 207 [M+]. 88 (100) |  | 1221 |  |  |  |  |  |  |  |  |  |  | 0.25 | 0.10 |
| 2-(2,6,6-trimethylcyclohexen-1-yl)acetaldehyde | C11H18O | 1245 |  |  | 0.32 | 0.07 | 0.05 | 0.06 | 0.09 | 0.08 | 0.04 | 0.11 | 0.18 | 0.07 |
| (E)-dec-2-enal | C10H18O | 1256 |  |  |  |  | 0.03 | 0.04 |  |  |  |  |  |  |
| 5-pentyl-3h-furan-2-one | C9H14O2 | 1262 |  |  |  |  |  |  |  |  |  |  | 0.08 | 0.03 |
| Unidentified m/z 191 [M+]. 84 (100) | C11H10 | 1271 |  |  |  |  |  |  |  |  |  |  | 0.20 | 0.08 |
| 1-сyclohexyl-2-buten-1-ol | C10H18O | 1277 |  |  |  |  |  |  |  |  |  |  | 0.13 | 0.05 |
| Unidentified m/z ? [M+], 56 (100) |  | 1283 |  |  |  |  | 0.04 | 0.05 |  |  |  |  |  |  |
| nonanoic acid | C9H18O2 | 1294 |  |  |  |  | 0.08 | 0.09 |  |  |  |  |  |  |
| ***5-methyl-2-propan-2-ylphenol;* [*Thymol*]** | **C10H14O** | ***1300*** |  |  | ***1.95*** | ***0.42*** |  |  |  |  |  |  |  |  |
| 4-ethenyl-2-methoxyphenol | C9H10O2 | 1309 |  |  |  |  | 0.14 | 0.17 |  |  | 0.08 | 0.22 | 0.33 | 0.13 |
| 1,1,6-trimethyl-2H-naphthalene | C13H16 | 1341 |  |  |  |  | 0.08 | 0.10 | 0.05 | 0.04 | 0.04 | 0.11 | 0.10 | 0.04 |
| 1,4,4,7a-tetramethyl-5H-indene | C13H18 | 1346 |  |  |  |  |  |  |  |  | 0.02 | 0.06 |  |  |
| 4,4,7-trimethyl-2,3-dihydro-1H-naphthalene | C13H18 | 1348 |  |  |  |  | 0.01 | 0.02 |  |  |  |  |  |  |
| 2-methoxy-4-prop-2-enylphenol; [Eugenol]  | C10H12O2 | 1358 |  |  |  |  | 0.03 | 0.03 |  |  |  |  |  |  |
| (E)-undec-2-enal | C11H20O | 1368 |  |  |  |  | 0.05 | 0.06 |  |  |  |  |  |  |
| (Z)-2-butyloct-2-enal | C12H22O | 1379 |  |  |  |  | 0.12 | 0.14 |  |  |  |  |  |  |
| 1-(2,6,6-trimethylcyclohexa-1,3-dien-1-yl)but-2-en-1-one; [β-Damascenone]  | C13H18O | 1380 |  |  |  |  |  |  | 0.14 | 0.12 | 0.04 | 0.10 | 0.50 | 0.20 |
| Unidentified m/z ? [M+], 149 (100) |  | 1386 |  |  |  |  |  |  |  |  | 0.02 | 0.05 |  |  |
| decanoic acid | C10H20O2 | 1391 |  |  |  |  | 0.11 | 0.13 |  |  |  |  |  |  |
| (E)-tetradec-7-ene | C14H28 | 1394 | 0.09 | 0.03 |  |  |  |  | 0.08 | 0.07 | 0.02 | 0.05 | 0.10 | 0.04 |
| 4,5-diethyl-2,2-dimethyl-3-prop-1-en-2-yl-1,2,5-oxasilaborole | C11H21BOSi | 1394 |  |  | 0.15 | 0.03 |  |  |  |  |  |  |  |  |
| ***tetradecane*** | **C14H30** | ***1400*** | ***2.05*** | ***0.66*** | ***1.05*** | ***0.23*** | ***0.04*** | ***0.04*** | ***0.44*** | ***0.38*** | ***0.15*** | ***0.40*** | ***0.83*** | ***0.33*** |
| 6,10-dimethylundecan-2-one | C13H26O | 1405 |  |  |  |  |  |  | 0.12 | 0.11 | 0.01 | 0.04 |  |  |
| [(2S,7aR)-4,4,7a-trimethyl-2,5,6,7-tetrahydro-1-benzofuran-2-yl]methanol | C13H20O | 1411 |  |  |  |  |  |  | 0.07 | 0.06 |  |  |  |  |
| 4-(2,6,6-trimethylcyclohexa-1,3-dien-1-yl)butan-2-one | C13H20O | 1412 |  |  |  |  |  |  |  |  | 0.01 | 0.04 | 0.05 | 0.02 |
| Unidentified m/z 208 [M+]. 73 (100) |  | 1415 |  |  |  |  |  |  |  |  |  |  | 0.13 | 0.05 |
| (E)-4-(2,6,6-trimethylcyclohex-2-en-1-yl)but-3-en-2-one ; [α-Ionone] | C13H20O | 1420 | 0.18 | 0.06 |  |  |  |  | 0.11 | 0.09 | 0.01 | 0.04 | 0.05 | 0.02 |
| (Z)-4-(2,6,6-trimethylcyclohex-2-en-1-yl)but-3-en-2-one | C13H20O | 1423 |  |  |  |  | 0.02 | 0.03 |  |  |  |  |  |  |
| (E)-4-(2,4,4-trimethylcyclohexa-1,5-dien-1-yl)but-3-en-2-one | C13H18O | 1424 |  |  |  |  |  |  | 0.04 | 0.03 | 0.03 | 0.08 | 0.15 | 0.06 |
| 6-methyl-6-(5-methylfuran-2-yl) heptan-2-one | C13H20O2 | 1428 |  |  |  |  |  |  | 0.03 | 0.02 | 0.01 | 0.03 | 0.08 | 0.03 |
| 2-(2,6-dimethylhept-6-en-2-yl)-5-methylfuran | C14H22O | 1449 |  |  |  |  |  |  |  |  | 0.01 | 0.03 |  |  |
| **(*5E*)*-6,10-dimethylundeca-5,9-dien-2-one;* [*Geranylacetone*]** | **C13H22O** | ***1454*** | ***1.46*** | ***0.47*** | ***1.24*** | ***0.27*** | ***0.18*** | ***0.22*** | ***0.47*** | ***0.40*** | ***0.12*** | ***0.32*** | ***0.43*** | ***0.17*** |
| (4Z)-4-(2,6,6-trimethylcyclohex-2-en-1-ylidene)butan-2-one | C13H20O | 1457 |  |  |  |  |  |  |  |  |  |  | 0.10 | 0.04 |
| 2,6-ditert-butylcyclohexa-2,5-diene-1,4-dione | C14H20O2 | 1457 |  |  |  |  |  |  | 0.05 | 0.05 |  |  |  |  |
| Unidentified m/z ? [M+], 121 (100) |  | 1464 |  |  |  |  |  |  | 0.05 | 0.05 |  |  |  |  |
| 2,6,10-trimethyltridecane | C16H34 | 1465 |  |  |  |  |  |  |  |  | 0.03 | 0.08 |  |  |
| 2,6-ditert-butyl-4-hydroxy-4-methylcyclohexa-2,5-dien-1-one | C15H24O2 | 1471 | 0.10 | 0.03 | 0.12 | 0.02 |  |  | 0.05 | 0.04 | 0.01 | 0.02 | 0.05 | 0.02 |
| **(*E)-4-*(*2,6,6-trimethylcyclohexen-1-yl*)*but-3-en-2-one;* [β*-Ionone*]** | **C13H20O** | ***1478*** | ***5.28*** | ***1.70*** | ***3.45*** | ***0.75*** | ***0.76*** | ***0.89*** | ***2.02*** | ***1.75*** | ***0.74*** | ***1.98*** | ***2.39*** | ***0.95*** |
| dibenzofuran | C12H8O | 1492 |  |  |  |  |  |  | 0.08 | 0.07 | 0.001 | 0.001 |  |  |
| 2,6,10-trimethyltetradecane | C17H36 | 1493 |  |  |  |  |  |  |  |  |  |  | 0.13 | 0.05 |
| pentadecane | C15H32 | 1500 | 0.16 | 0.05 |  |  | 0.02 | 0.03 | 0.11 | 0.10 | 0.02 | 0.05 | 0.13 | 0.05 |
| 2,6-ditert-butyl-4-methylphenol | C15H24O | 1504 | 0.20 | 0.07 |  |  |  |  | 0.04 | 0.04 | 0.02 | 0.04 | 0.03 | 0.01 |
| 4,4,7a-trimethyl-6,7-dihydro-5H-1-benzofuran-2-one; [dihydroactinidiolide] | C11H16O2 | 1508 | 0.24 | 0.08 |  |  |  |  | 0.14 | 0.12 | 0.05 | 0.14 | 0.15 | 0.06 |
| ***4-*[(*1R,2R*)*-2-methyl-3-oxocyclohexyl]butanal*** | **C11H18O2** | ***1511*** |  |  | ***1.51*** | ***0.33*** | ***0.22*** | ***0.26*** |  |  |  |  | ***0.33*** | ***0.13*** |
| Z-2,6,10-trimethylundeca-2,5,9-trien-4-one | C14H22O | 1511 | 0.71 | 0.23 |  |  |  |  | 0.14 | 0.12 | 0.09 | 0.23 |  |  |
| 8a-methyl-3,4,4a,5,6,7-hexahydro-2H-naphthalene-1,8-dione | C11H16O2 | 1515 | 0.60 | 0.19 |  |  | 0.05 | 0.06 | 0.21 | 0.18 | 0.19 | 0.52 | 0.65 | 0.26 |
| 1-methyl-8-propan-2-yl-1,2,3,4-tetrahydronaphthalene | C14H20 | 1524 |  |  |  |  |  |  |  |  |  |  | 0.20 | 0.08 |
| 1,1,3,3-tetramethylinden-2-one | C13H16O | 1524 |  |  |  |  |  |  | 0.02 | 0.02 | 0.01 | 0.04 |  |  |
| Unidentified m/z 218 [M+]. 135 (100) |  | 1533 |  |  |  |  |  |  |  |  |  |  | 0.08 | 0.03 |
| 2,6,6,9-tetramethyltricyclo[5.4.0.02,10]undec-8-en-11-one |  | 1541 | 0.24 | 0.08 |  |  |  |  |  |  | 0.01 | 0.04 |  |  |
| Unidentified m/z ? [M+], 57 (100) |  | 1541 |  |  |  |  |  |  | 0.03 | 0.03 |  |  |  |  |
| Unidentified m/z 281 [M+]. 119 (100) |  | 1542 |  |  |  |  |  |  |  |  |  |  | 0.10 | 0.04 |
| Unidentified m/z ? [M+], 97 (100) |  | 1542 |  |  |  |  |  |  | 0.02 | 0.02 |  |  |  |  |
| 9H-fluorene | C13H10 | 1547 |  |  |  |  |  |  |  |  |  |  | 0.05 | 0.02 |
| (6E)-3,7,11-trimethyldodeca-1,6,10-trien-3-ol; [Nerolidol] | C15H26O | 1555 |  |  |  |  | 0.01 | 0.02 | 0.02 | 0.02 | 0.02 | 0.05 |  |  |
| 1,2,4-trimethoxy-5-prop-1-enylbenzene | C12H16O3 | 1555 |  |  | 0.21 | 0.04 |  |  |  |  |  |  |  |  |
| Unidentified m/z 208 [M+], 208 (100) |  | 1556 |  |  |  |  |  |  | 0.03 | 0.03 |  |  |  |  |
| Unidentified m/z 280 [M+], 71 (100) |  | 1561 |  |  |  |  |  |  | 0.06 | 0.05 | 0.01 | 0.03 |  |  |
| 3-methylpentadecane | C16H34 | 1565 |  |  |  |  |  |  | 0.03 | 0.03 | 0.01 | 0.03 | 0.08 | 0.03 |
| (E)-2-methyl-4-(2,6,6-trimethylcyclohexen-1-yl)but-2-enal | C14H22O | 1569 |  |  | 0.20 | 0.04 |  |  | 0.06 | 0.05 | 0.03 | 0.09 | 0.08 | 0.03 |
| 2,2,7,7-tetramethyltricyclo[6.2.1.01,6]undec-5-en-4-one | C15H22O | 1570 |  |  |  |  | 0.03 | 0.04 |  |  |  |  |  |  |
| (3E,5E)-6,10-dimethylundeca-3,5,9-trien-2-one; [Pseudoionone] | C13H20O | 1581 |  |  | 0.27 | 0.06 |  |  | 0.05 | 0.04 | 0.02 | 0.04 |  |  |
| dodecanoic acid | C12H24O2 | 1582 |  |  |  |  | 0.21 | 0.24 | 0.03 | 0.02 | 0.04 | 0.11 | 0.20 | 0.08 |
| tricyclo[10.2.1.02,11]pentadeca-4,8-diene | C15H22 | 1593 |  |  |  |  |  |  |  |  |  |  | 0.63 | 0.25 |
| 3-O-heptan-2-yl 1-O-(2-methylpropyl) propanedioate | C14H26O4 | 1594 |  |  |  |  | 0.03 | 0.03 |  |  |  |  |  |  |
| hexadecane | C16H34 | 1600 | 0.71 | 0.23 | 0.97 | 0.21 | 0.02 | 0.02 | 0.31 | 0.27 | 0.23 | 0.62 | 0.98 | 0.39 |
| Unidentified m/z 224 [M+]. 69 (100) |  | 1651 |  |  |  |  |  |  |  |  |  |  | 0.15 | 0.06 |
| tributyl phosphate | C12H27O4P | 1662 |  |  |  |  | 0.04 | 0.05 | 0.11 | 0.09 | 0.02 | 0.05 |  |  |
| 1-((1E,3E)-hepta-1,3-dien-1-yl)-3,7,7-trimethyl-2-oxabicyclo[3.2.0]hept-3-ene | C16H24O | 1668 |  |  |  |  |  |  |  |  | 0.01 | 0.03 |  |  |
| Unidentified m/z 236 [M+], 57 (100) |  | 1675 |  |  |  |  |  |  | 0.13 | 0.11 | 0.04 | 0.10 |  |  |
| **(*E*)*-heptadec-8-ene*** | **C17H34** | ***1677*** | ***0.19*** | ***0.06*** |  |  |  |  | ***1.18*** | ***1.02*** | ***0.03*** | ***0.08*** |  |  |
| 2-tetradecyloxirane | C16H32O | 1677 |  |  |  |  |  |  |  |  |  |  | 0.13 | 0.05 |
| hexadecanal |  C16H32O | 1679 |  |  | 0.74 | 0.16 | 0.25 | 0.30 |  |  |  |  |  |  |
| tetradecan-1-ol | C14H30O | 1685 | 0.36 | 0.12 |  |  |  |  | 0.63 | 0.54 | 0.08 | 0.22 |  |  |
| heptadec-1-ene | C17H34 | 1686 |  |  |  |  |  |  |  |  |  |  | 0.13 | 0.05 |
| (Z)-pentadec-11-enal | C15H28O | 1689 |  |  |  |  |  |  |  |  | 0.11 | 0.29 |  |  |
| ***heptadecane*** | **C17H36** | ***1700*** | ***0.81*** | ***0.26*** | ***1.29*** | ***0.28*** | ***0.06*** | ***0.07*** | ***1.74*** | ***1.50*** | ***0.17*** | ***0.47*** | ***0.55*** | ***0.22*** |
| 2,6,10,14-tetramethylhexadecane; [Phytane] | C20H42 | 1705 |  |  |  |  |  |  |  |  |  |  | 0.28 | 0.11 |
| ***pentadecanal*** | **C15H30O** | ***1712*** | ***2.12*** | ***0.68*** | ***1.38*** | ***0.30*** | ***1.27*** | ***1.50*** | ***1.79*** | ***1.55*** | ***0.56*** | ***1.50*** | ***1.53*** | ***0.61*** |
| 4a,8,8-trimethyl-1,1a,4,5,6,7-hexahydrocyclopropa[j]naphthalene-2-carbaldehyde; [Thujopsenal] | C15H22O | 1731 |  |  |  |  |  |  |  |  | 0.01 | 0.03 |  |  |
| tetradecan-3-ol | C14H30O | 1733 |  |  |  |  | 0.09 | 0.11 |  |  |  |  |  |  |
| (2E,6E)-3,7,11-trimethyldodeca-2,6,10-trienal; [Farnesal] | C15H24O | 1737 |  |  |  |  |  |  | 0.10 | 0.08 | 0.02 | 0.05 |  |  |
| phenanthrene | C14H10 | 1744 | 0.75 | 0.24 | 0.85 | 0.18 | 0.04 | 0.04 | 0.25 | 0.21 | 0.10 | 0.28 | 0.28 | 0.11 |
| benzyl benzoate | C14H12O2 | 1750 |  |  |  |  | 0.03 | 0.04 | 0.10 | 0.08 | 0.03 | 0.09 | 0.35 | 0.14 |
| (1R,4R)-3,3,4-trimethyl-4-(4-methylphenyl)cyclopentan-1-ol | C15H22O | 1768 | 0.40 | 0.13 |  |  |  |  | 0.15 | 0.13 | 0.06 | 0.16 | 0.20 | 0.08 |
| ***tetradecanoic acid*** | **C14H28O2** | ***1776*** |  |  | ***2.94*** | ***0.64*** | ***1.52*** | ***1.80*** | ***2.46*** | ***2.12*** | ***4.11*** | ***11.05*** | ***2.29*** | ***0.91*** |
| methyl (7E,10E,13E)-hexadeca-7,10,13-trienoate | C17H28O2 | 1788 |  |  |  |  | 0.02 | 0.02 |  |  |  |  |  |  |
| 2-methylheptadecane |  C18H38 | 1798 | 0.56 | 0.18 |  |  |  |  |  |  |  |  |  |  |
| octadecane | C18H38 | 1799 |  |  |  |  |  |  |  |  |  |  | 0.33 | 0.13 |
| dodecan-2-ylbenzene | C18H30 | 1802 |  |  |  |  | 0.03 | 0.04 |  |  |  |  |  |  |
| 1,4a-dimethyl-7-propan-2-yl-2,3,4,9,10,10a-hexahydro-1H-phenanthrene | C19H28 | 1803 |  |  |  |  |  |  |  |  |  |  | 0.13 | 0.05 |
| tetradecanal | C16H32O | 1814 | 0.15 | 0.05 |  |  |  |  | 0.16 | 0.13 | 0.02 | 0.05 |  |  |
| 3,3,4,5,5,8-hexamethyl-6,7-dihydro-2H-s-indacen-1-one | C18H24O | 1814 |  |  |  |  | 0.03 | 0.04 |  |  |  |  |  |  |
| hexadecanal | C14H28O | 1826 |  |  |  |  | 0.16 | 0.19 |  |  |  |  | 0.15 | 0.06 |
| ***6,10,14-trimethylpentadecan-2-one*** | **C18H36O** | ***1847*** | ***4.25*** | ***1.37*** | ***2.26*** | ***0.49*** | ***0.44*** | ***0.52*** | ***3.70*** | ***3.20*** | ***1.40*** | ***3.77*** | ***2.31*** | ***0.92*** |
| (Z)-octadec-9-en-1-ol  | C20H40O | 1853 |  |  |  |  | 0.09 | 0.11 |  |  |  |  |  |  |
| pentadec-14-enoic acid | C15H28O2 | 1863 |  |  |  |  | 0.24 | 0.29 |  |  | 0.13 | 0.35 |  |  |
| bis(2-methylpropyl) benzene-1,2-dicarboxylate; [diisobutyl phthalate] | C16H22O4 | 1869 |  |  | 1.12 | 0.24 |  |  |  |  |  |  |  |  |
| benzyl 2-hydroxybenzoate | C14H12O3 | 1869 |  |  |  |  | 0.08 | 0.09 |  |  |  |  |  |  |
| (4aS,7S)-7-ethenyl-1,1,4a,7-tetramethyl-3,4,4b,5,6,9,10,10a-octahydro-2H-phenanthrene | C20H32 | 1881 |  |  | 0.11 | 0.02 |  |  |  |  |  |  |  |  |
| ***1-hexadecanol*** | **C16H34O** | ***1888*** |  |  |  |  |  |  |  |  |  |  | ***4.47*** | ***1.78*** |
| ***pentadecanoic acid*** | **C15H30O2** | ***1889*** |  |  |  |  | ***0.10*** | ***0.12*** | ***6.48*** | ***5.59*** | ***1.38*** | ***3.70*** |  |  |
| ***heptadecan-1-ol*** | **C17H36O** | ***1890*** | ***3.24*** | ***1.04*** |  |  | ***4.37*** | ***5.17*** | ***2.46*** | ***2.12*** | ***1.69*** | ***4.55*** |  |  |
| ***2-methylhexadecan-1-ol*** | **C16H34O** | ***1893*** |  |  | ***1.29*** | ***0.28*** |  |  |  |  |  |  |  |  |
| **(*7Z,10Z,13Z*)*-hexadeca-7,10,13-trienal*** | **C16H26O** | ***1895*** |  |  |  |  | ***0.67*** | ***0.79*** |  |  |  |  | ***1.41*** | ***0.56*** |
| nonadecane | C19H40 | 1900 |  |  |  |  | 0.29 | 0.35 | 0.49 | 0.42 | 0.37 | 0.99 | 0.73 | 0.29 |
| 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione  | C17H24O3 | 1911 |  |  |  |  |  |  |  |  |  |  | 0.20 | 0.08 |
| **(*5E,9E*)*-6,10,14-trimethylpentadeca-5,9,13-trien-2-one*** | **C18H30O** | ***1916*** | ***1.82*** | ***0.59*** | ***1.40*** | ***0.30*** | ***0.37*** | ***0.43*** |  |  |  |  |  |  |
| **(*4aS,4bS,7R,10aS*)*-7-ethenyl-1,1,4a,7-tetramethyl-3,4,4b,5,6,9,10,10a-octahydro-2H-phenanthrene;* [*Sandaracopimaradiene*]** | **C20H32** | ***1916*** |  |  |  |  |  |  | ***1.62*** | ***1.40*** | ***2.40*** | ***6.44*** |  |  |
| **(*4aS,8S,8aS)-4,4,8a-trimethyl-7-methylidene-8-*[(*2E*)*-3-methylpenta-2,4-dienyl]-2,3,4a,5,6,8-hexahydro-1H-naphthalene;* [*Biformene*]** | **C20H32** | ***1918*** |  |  |  |  |  |  |  |  |  |  | ***2.44*** | ***0.97*** |
| 1-(5,5,8a-trimethyl-2-methylidene-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl)-3-methylpentan-3-ol | C20H36O | 1931 |  |  |  |  | 0.27 | 0.32 |  |  |  |  |  |  |
| (E)-6-methyl-8-(2,6,6-trimethylcyclohexen-1-yl)oct-5-en-2-one | C18H30O | 1938 |  |  |  |  |  |  |  |  |  |  | 0.23 | 0.09 |
| (4aS,4bS,7R,10aS)-7-ethenyl-1,1,4a,7-tetramethyl-3,4,4b,5,6,9,10,10a-octahydro-2H-phenanthrene; [Sandaracopimaradiene, isomer]  | C20H33 | 1941 |  |  |  |  |  |  | 0.47 | 0.41 | 0.60 | 1.62 |  |  |
| 3,7,11,15-tetramethylhexadec-1-en-3-ol; [Isophytol] | C20H40O | 1952 | 0.23 | 0.07 |  |  |  |  | 0.30 | 0.26 | 0.15 | 0.39 |  |  |
| 5,5,9,13-tetramethylpentacyclo[11.2.1.01,10.04,9.012,14]hexadecane; [Trachylobane] | C20H32 | 1959 |  |  |  |  |  |  | 0.47 | 0.40 |  |  |  |  |
| (Z)-hexadec-11-enoic acid; [Tanacetumoleic acid] | C16H30O2 | 1959 |  |  |  |  | 4.90 | 5.80 |  |  | 0.27 | 0.72 | 0.60 | 0.24 |
| **(*2S,4aS,4bS,8aS*)*-2-ethenyl-2,4b,8,8-tetramethyl-3,4,4a,5,6,7,8a,9-octahydro-1H-phenanthrene;* [*Isopimaradiene*]** |  **C20H32** | ***1970*** | ***1.60*** | ***0.52*** | ***1.50*** | ***0.32*** |  |  | ***1.35*** | ***1.17*** |  |  | ***2.39*** | ***0.95*** |
| ***hexadecanoic acid*** | **C16H32O2** | ***1985*** | ***0.99*** | ***0.32*** | ***2.94*** | ***0.64*** | ***9.97*** | ***11.80*** | ***13.55*** | ***11.70*** | ***11.96*** | ***32.14*** | ***3.09*** | ***1.23*** |
| **(*3R,4aR,6aS,10aS,10bR*)*-3-ethenyl-3,4a,7,7,10a-pentamethyl-2,5,6,6a,8,9,10,10b-octahydro-1H-benzo[f]chromene;* [*Manoyl oxide*]** | **C20H34O** | ***1993*** |  |  |  |  |  |  |  |  |  |  | ***1.28*** | ***0.51*** |
| (2S,4aR,4bS,10aR)-2-ethenyl-2,4a,8,8-tetramethyl-3,4,4b,5,6,7,10,10a-octahydro-1H-phenanthrene; [Rimuene] | C20H32 | 2003 |  |  |  |  |  |  |  |  |  |  | 0.55 | 0.22 |
| kaur-16-ene; [Kaurene] | C20H32 | 2011 |  |  |  |  |  |  |  |  |  |  | 0.68 | 0.27 |
| octadecanal | C18H36O | 2026 |  |  |  |  | 0.16 | 0.19 |  |  |  |  | 0.15 | 0.06 |
| (6E,10E)-3,7,11,15-tetramethylhexadeca-1,6,10,14-tetraen-3-ol; [Geranyl linalool isomer] | C20H34O | 2033 |  |  |  |  | 0.09 | 0.10 |  |  |  |  | 0.13 | 0.05 |
| ***5-*(*5,5,8a-trimethyl-2-methylidene-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl*)*-3-methylpent-1-en-3-ol*** | **C20H34O** | ***2042*** |  |  | ***9.35*** | ***2.02*** |  |  |  |  |  |  |  |  |
| ***Manool; [(3R)-5-*[(*1S,4aS,8aS*)*-5,5,8a-trimethyl-2-methylidene-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl]-3-methylpent-1-en-3-ol*]** | **C20H34O** | ***2043*** | ***0.89*** | ***0.29*** |  |  |  |  | ***4.39*** | ***3.79*** | ***16.44*** | ***44.18*** | ***6.43*** | ***2.56*** |
| ***(5S,8S,9S,10R,13S,14S)-10,13-dimethyl-5,6,7,8,9,12,14,15,16,17-decahydro-4H-cyclopenta[a]phenanthrene-3,11-dione*** | **C19H26O2** | ***2065*** | ***0.62*** | ***0.20*** |  |  |  |  |  |  | ***2.54*** | ***6.84*** |  |  |
| **(*3S,5R,8S,9S,10R,13S,14S*)*-4,4,10,13-tetramethyl-1,2,3,5,6,7,8,9,11,12,14,15,16,17-tetradecahydrocyclopenta[a]phenanthren-3-ol*** | **C21H36O** | ***2065*** |  |  |  |  |  |  | ***2.33*** | ***2.02*** |  |  | ***2.99*** | ***1.19*** |
| ***octadecan-1-ol*** | **C18H38O** | ***2090*** |  |  |  |  | ***1.33*** | ***1.58*** |  |  |  |  | ***0.65*** | ***0.26*** |
| ***henicosane*** | **C21H44** | ***2100*** | ***1.43*** | ***0.46*** |  |  | ***3.13*** | ***3.70*** | ***1.84*** | ***1.59*** | ***1.43*** | ***3.85*** | ***1.86*** | ***0.74*** |
| 2,4,6-tritert-butylbenzoic acid | C19H30O2 | 2106 |  |  |  |  |  |  |  |  | 0.62 | 1.66 |  |  |
| ***3,7,11,15-tetramethylhexadec-2-en-1-ol;* [*Phytol*]** | **C20H40O** | ***2118*** | ***2.19*** | ***0.70*** |  |  | ***10.08*** | ***11.93*** | ***3.28*** | ***2.83*** | ***6.40*** | ***17.20*** | ***2.36*** | ***0.94*** |
| ***methyl octadecanoate*** | **C19H38O2** | ***2129*** |  |  |  |  |  |  | ***1.20*** | ***1.04*** | ***1.09*** | ***2.92*** | ***2.69*** | ***1.07*** |
| ***1,1-diprop-2-enoxytetradecane*** | **C20H38O2** | ***2140*** |  |  |  |  |  |  | ***1.02*** | ***0.88*** |  |  |  |  |
| **(*9Z,12Z*)*-octadeca-9,12-dienoic acid;* [*Linoleic acid*]** | **C18H32O2** | ***2141*** | ***0.30*** | ***0.10*** |  |  |  |  |  |  | ***3.14*** | ***8.44*** |  |  |
| **(*9Z,12Z,15Z*)*-octadeca-9,12,15-trienoic acid;* [*Linolenic acid*]** | **C18H30O2** | ***2173*** |  |  |  |  | ***18.41*** | ***21.79*** |  |  |  |  |  |  |
| ***nonadeca-1,18-diene-7,10-dione*** | **C19H32O2** | ***2175*** | ***0.85*** | ***0.27*** |  |  | ***1.10*** | ***1.30*** | ***0.78*** | ***0.67*** | ***1.40*** | ***3.75*** | ***0.65*** | ***0.26*** |
| 7-ethenyl-1,4a,7-trimethyl-3,4,4b,5,6,8,10,10a-octahydro-2H-phenanthrene-1-carbaldehyde | C20H30O | 2188 |  |  |  |  |  |  | 0.35 | 0.31 |  |  |  |  |
| docosane | C22H46 | 2200 |  |  |  |  | 0.36 | 0.42 |  |  |  |  |  |  |
| 7a,8a,10a-trimethylhexadecahydro-1h-cyclopenta[7,8]phenanthro[2,3-b]oxiren-1-ol | C20H32O2 | 2203 |  |  | 0.62 | 0.13 |  |  |  |  |  |  |  |  |
| 7-ethenyl-1,1,4a,7-tetramethyl-3,4,4b,5,6,8,10,10a-octahydrophenanthren-2-one  | C20H30O | 2206 |  |  |  |  |  |  | 0.95 | 0.82 |  |  | 0.35 | 0.14 |
| (Z)-icos-9-en-1-ol | C20H40O | 2231 |  |  |  |  | 0.51 | 0.60 |  |  |  |  |  |  |
| ***1-*[(*8R,9S,10S,13S,14S,17S*)*-3-hydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]ethanone*;[*Allopregnanolon*e]** | **C21H34O2** | ***2243*** | ***0.82*** | ***0.26*** | ***7.59*** | ***1.64*** | ***0.73*** | ***0.87*** |  |  |  |  |  |  |
| ***1-*[(*3R,5R,8R,9S,10S,13S,14S,17S*)*-3-hydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta*[*a*]*phenanthren-17-yl]ethanone;* [*Pregnanolone*]** | **C21H34O2** | ***2244*** |  |  |  |  |  |  |  |  |  |  | ***4.12*** | ***1.64*** |
| **(*8R,9S,10R,13S,14S*)*-10,13-dimethyl-1,2,7,8,9,11,12,14,15,16-decahydrocyclopenta*[*a*]*phenanthrene-3,6,17-trione*** | **C19H24O3** | ***2244*** |  |  |  |  |  |  | ***7.90*** | ***6.81*** | ***13.13*** | ***35.29*** |  |  |
| (1R,2R,4aS,8aS)-1-[(3R)-3-hydroxy-3-methylpent-4-enyl]-2,5,5,8a-tetramethyl-3,4,4a,6,7,8-hexahydro-1H-naphthalen-2-ol; [Sclareol] | C20H36O2 | 2246 |  |  |  |  | 0.20 | 0.24 |  |  |  |  |  |  |
| **[(*1R,4aR,4bS,7R,10aR*)*-7-ethenyl-1,4a,7-trimethyl-3,4,4b,5,6,9,10,10a-octahydro-2H-phenanthren-1-yl]methanol*;[*Sandaracopimarinol*]** | **C20H32O** | ***2279*** |  |  |  |  |  |  | ***1.21*** | ***1.04*** |  |  |  |  |
| ***tricosane*** | **C23H48** | ***2300*** | ***2.55*** | ***0.82*** | ***0.77*** | ***0.17*** | ***10.79*** | ***12.77*** | ***1.37*** | ***1.18*** | ***3.80*** | ***10.22*** | ***1.13*** | ***0.45*** |
| ***1-*[(*5R,8R,9S,10S,13R,14S,17S*)*-13-(hydroxymethyl*)*-10-methyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta*[*a*]*phenanthren-17-yl]ethanol***  | **C21H36O2** | ***2316*** |  |  |  |  |  |  | ***0.84*** | ***0.73*** | ***1.64*** | ***4.42*** | ***1.08*** | ***0.43*** |
| **(*E*)*-8-(2,5,5,8a-tetramethyl-1,4,4a,6,7,8-hexahydronaphthalen-1-yl*)*-6-methyloct-5-en-2-ol*** | **C23H40O** | ***2326*** |  |  | ***8.99*** | ***1.94*** | ***0.64*** | ***0.75*** | ***2.93*** | ***2.53*** | ***2.64*** | ***7.10*** | ***1.03*** | ***0.41*** |
| cyclopenta[a]phenanthrene, perhydro-17-acetoxy-1-hydroxy-4,10,13-trimethyl | C22H36O3 | 2383 |  |  |  |  |  |  | 0.19 | 0.17 | 0.06 | 0.15 |  |  |
| methyl (E)-5-[5-(hydroxymethyl)-5,8a-dimethyl-2-methylidene-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl]-3-methylpent-2-enoate | C21H34O3 | 2396 |  |  |  |  |  |  | 0.24 | 0.20 | 0.63 | 1.70 | 0.20 | 0.08 |
| ***1-*[(*8S,9S,10S,13S,14S,17S*)*-3,11-dihydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta*[*a*]*phenanthren-17-yl]ethanone*** | **C21H34O3** | ***2409*** | ***0.53*** | ***0.17*** |  |  |  |  | ***1.90*** | ***1.64*** | ***1.12*** | ***3.00*** | ***1.41*** | ***0.56*** |
| (2S,3aR,5aS,9aS,9bR)-3a,4',6,6,9a-pentamethylspiro[1,4,5,5a,7,8,9,9b-octahydrobenzo[e][1]benzofuran-2,5'-furan]-2'-one | C20H30O3 | 2423 |  |  |  |  | 0.83 | 0.99 |  |  |  |  |  |  |
| (Z)-docos-13-en-1-ol(Z)-докоз-13-ен-1-ол | C22H44O | 2433 |  |  |  |  | 0.20 | 0.24 |  |  |  |  |  |  |
| **[*(8R,9S,10R,13S,14S*)*-4,10,13-trimethyl-3-oxo-1,2,6,7,8,9,11,12,14,15,16,17-dodecahydrocyclopenta*[*a*]*phenanthren-17-yl*] *acetate*** | **C22H32O3** | ***2467*** | ***0.37*** | ***0.12*** | ***5.20*** | ***1.12*** |  |  | ***0.77*** | ***0.67*** | ***0.88*** | ***2.37*** | ***0.28*** | ***0.11*** |
| ***pentacosane*** | **C25H52** | ***2500*** | ***2.14*** | ***0.69*** | ***1.33*** | ***0.29*** | ***8.73*** | ***10.34*** | ***0.50*** | ***0.43*** | ***3.80*** | ***10.20*** | ***0.50*** | ***0.20*** |
| **[(*1S,2R,5S,7R,9S,11S,12S,15S,16S*)*-15-acetyl-2,16-dimethyl-8-oxapentacyclo*[*9.7.0.02,7.07,9.012,16*]*octadecan-5-yl*] *acetate*** | **C23H34O4** | ***2544*** | ***3.66*** | ***1.18*** |  |  |  |  | ***2.68*** | ***2.31*** | ***1.92*** | ***5.17*** |  |  |
| hexacosane | C26H54 | 2600 |  |  |  |  | 0.20 | 0.24 |  |  |  |  |  |  |
| tetracosanal | C24H48O | 2635 |  |  |  |  | 0.05 | 0.06 |  |  |  |  |  |  |
| heptacos-1-ene | C27H54 | 2677 |  |  |  |  |  |  |  |  | 0.08 | 0.23 |  |  |
| ***pentacosan-1-ol*** | **C25H52O** | ***2685*** |  |  |  |  | ***2.27*** | ***2.68*** |  |  |  |  |  |  |
| ***heptacosane*** | **C27H56** | ***2698*** | ***0.54*** | ***0.17*** |  |  | ***2.16*** | ***2.55*** |  |  | ***0.79*** | ***2.13*** | ***0.15*** | ***0.06*** |
| ***(3-acetyloxy-10,13-dimethyl-1-oxo-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydrocyclopenta[a]phenanthren-17-yl) acetate*** | **C23H34O5** | ***2711*** |  |  |  |  |  |  | ***0.83*** | ***0.72*** | ***1.06*** | ***2.84*** |  |  |
| ***(3S,5S,8R,9S,10S,13R,17R)-17-[(E,2R,5S)-5,6-dimethylhept-3-en-2-yl]-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-yl] acetate*** | **C30H50O2** | ***2712*** |  |  | ***2.78*** | ***0.60*** | ***1.00*** | ***1.18*** |  |  |  |  | ***0.15*** | ***0.06*** |
| bis(2-ethylhexyl) benzene-1,3-dicarboxylate | C24H38O4 | 2749 |  |  |  |  | 0.03 | 0.03 |  |  |  |  |  |  |
| **(*6E,10E,14E,18E*)*-2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene; [Squalene]*** | **C30H50** | ***2822*** | ***1.94*** | ***0.62*** | ***2.06*** | ***0.45*** | ***0.07*** | ***0.08*** | ***0.60*** | ***0.52*** | ***0.18*** | ***0.47*** | ***0.60*** | ***0.24*** |
| ***hexacosan-1-ol*** | **C26H54O** | ***2878*** |  |  |  |  | ***2.28*** | ***2.70*** |  |  |  |  |  |  |
| nonacosane | C29H60 | 2900 |  |  |  |  | 0.21 | 0.24 |  |  |  |  |  |  |
| **TOTAL** |  |  | **100.00** | **32.14** | **100.00** | **21.60** | **100.00** | **118.37** | **100.00** | **86.31** | **100.00** | **268.69** | **100.0** | **39.80** |

*Note:* for some compounds, trivial or most commonly used names are given in square brackets; Major compounds are highlighted in bold italics, the proportion of which, at least in one sample, exceeded 1%