
Access from the University of Nottingham repository:
http://eprints.nottingham.ac.uk/14452/3/Appendix_A_Final.pdf

Copyright and reuse:

The Nottingham ePrints service makes this work by researchers of the University of Nottingham available open access under the following conditions.

This article is made available under the University of Nottingham End User licence and may be reused according to the conditions of the licence. For more details see:
http://eprints.nottingham.ac.uk/end_user_agreement.pdf

For more information, please contact eprints@nottingham.ac.uk
## Appendix A

A list of reported metabolites found in human apocrine sweat secretions. For further information see Appendix A on the attached CD

<table>
<thead>
<tr>
<th>Components</th>
<th>Structure</th>
<th>Molecule</th>
<th>Mass</th>
<th>M+H</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>3-Hydroxy acids</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3-Hydroxy-3-methylhexanoic acid</td>
<td></td>
<td>C7H14O3</td>
<td>146.0943</td>
<td>147.1021</td>
</tr>
<tr>
<td>3-Hydroxy-4-methylhexanoic acid</td>
<td></td>
<td>C7H14O3</td>
<td>146.0943</td>
<td>147.1021</td>
</tr>
<tr>
<td>3-Hydroxy-3-methylheptanoic acid</td>
<td></td>
<td>C8H16O3</td>
<td>160.1099</td>
<td>161.0628</td>
</tr>
<tr>
<td>3-Hydroxy-4-methylheptanoic acid</td>
<td></td>
<td>C8H16O3</td>
<td>160.1099</td>
<td>161.0628</td>
</tr>
<tr>
<td>3-Hydroxyoctanoic acid</td>
<td></td>
<td>C8H16O3</td>
<td>160.1099</td>
<td>161.0628</td>
</tr>
<tr>
<td>3-Hydroxy-3-methyloctanoic acid</td>
<td></td>
<td>C9H18O3</td>
<td>174.1256</td>
<td>175.1334</td>
</tr>
<tr>
<td>3-Hydroxy-4-methyloctanoic acid</td>
<td></td>
<td>C9H18O3</td>
<td>174.1256</td>
<td>175.1334</td>
</tr>
<tr>
<td>3-Hydroxy-4-methylnonanoic acid</td>
<td></td>
<td>C10H20O3</td>
<td>188.1412</td>
<td>189.1491</td>
</tr>
<tr>
<td>3-Hydroxydecanoic acid</td>
<td></td>
<td>C10H20O3</td>
<td>188.1412</td>
<td>189.1491</td>
</tr>
<tr>
<td><strong>Unsaturated acids</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(Z)-3-Methylhex-2-enoic acid</td>
<td></td>
<td>C7H12O2</td>
<td>128.0837</td>
<td>129.0916</td>
</tr>
<tr>
<td>(E)-3-Methylhex-2-enoic acid</td>
<td></td>
<td>C7H12O2</td>
<td>128.0837</td>
<td>129.0916</td>
</tr>
<tr>
<td>4-Methyloct-4-enoic acid</td>
<td></td>
<td>C9H16O2</td>
<td>156.1150</td>
<td>157.1229</td>
</tr>
<tr>
<td>(Z)-4-Methyloct-3-enoic acid</td>
<td></td>
<td>C9H16O2</td>
<td>156.1150</td>
<td>157.1229</td>
</tr>
<tr>
<td>(E)-4-Methyloct-3-enoic acid</td>
<td></td>
<td>C9H16O2</td>
<td>156.1150</td>
<td>157.1229</td>
</tr>
<tr>
<td>(Z)-4-Methylnon-3-enoic acid</td>
<td></td>
<td>C10H18O2</td>
<td>170.1307</td>
<td>171.1385</td>
</tr>
<tr>
<td>(E)-4-Methylnon-3-enoic acid</td>
<td></td>
<td>C10H18O2</td>
<td>170.1307</td>
<td>171.1385</td>
</tr>
<tr>
<td>(E)-3-Methyl-2-octenoic acid</td>
<td></td>
<td>C9H16O2</td>
<td>156.1150</td>
<td>157.1229</td>
</tr>
<tr>
<td>(E)-3-Methyl-2-pentenoic acid</td>
<td></td>
<td>C6H10O2</td>
<td>114.0681</td>
<td>115.0759</td>
</tr>
<tr>
<td>(Z)-3-Methylhex-2-enoic acid</td>
<td></td>
<td>C7H12O2</td>
<td>128.0837</td>
<td>129.0916</td>
</tr>
</tbody>
</table>
7-Octenoic acid

9-Decenoic acid

10-Undecenoic acid

2-Hexenoic acid

9-Pentadecenoic acid

9-Hexadecenoic acid

9-Heptadecenoic acid

Oleic acid

Unsaturated C11 acid (10-undecenoic acid)

Steroidal

5α-Androst-16-en-3α-ol

Androsta-4, 16-dien-3-one

5α-Androst-16-en-3-one

Androsta-4, 16-dien-3α-ol

5α-Androst-16-en-3β-ol

5α-Androsta-5, 16-dien-3β-ol

Androst-5-ene-3β,17α/β-diols
Androsta-5, 16-dien-3β-ol  
\[
\text{C}_{19}\text{H}_{28}\text{O} \\
272.2140 \\
273.2218
\]

Androsta-5, 16-dien-3-one  
\[
\text{C}_{19}\text{H}_{26}\text{O} \\
270.1984 \\
271.2062
\]

Androsta-4, 16-dien-3β-ol  
\[
\text{C}_{19}\text{H}_{28}\text{O} \\
272.2140 \\
273.2218
\]

Cholesterol  
\[
\text{C}_{27}\text{H}_{46}\text{O} \\
386.3549 \\
387.3627
\]

Squalene  
\[
\text{C}_{30}\text{H}_{50} \\
410.3913 \\
411.3991
\]

5α-Dihydrotestosterone  
\[
\text{C}_{19}\text{H}_{30}\text{O}_{2} \\
290.2246 \\
291.2324
\]

5β-Dihydrotestosterone  
\[
\text{C}_{19}\text{H}_{30}\text{O}_{2} \\
290.2246 \\
291.2324
\]

Dehydroepiandrosterone  
\[
\text{C}_{19}\text{H}_{28}\text{O}_{2} \\
288.2089
\]

Testosterone  
\[
\text{C}_{19}\text{H}_{28}\text{O}_{2} \\
288.2089 \\
289.2168
\]

17-Oxo-5α-androstan-3β-yl sulfate  
\[
\text{C}_{19}\text{H}_{30}\text{O}_{5}\text{S} \\
370.1814 \\
371.1892
\]

17-Oxo-5-androsten-3β-yl sulfate  
\[
\text{C}_{19}\text{H}_{28}\text{O}_{5}\text{S} \\
368.1657 \\
369.1736
\]

Sulfanylalkanols  

3-Sulfanylhexan-1-ol  
\[
\text{C}_{6}\text{H}_{14}\text{OS} \\
134.0765 \\
135.0844
\]
### Amino acids degradation products and miscellaneous acids

<table>
<thead>
<tr>
<th>Name</th>
<th>Chemical Formula</th>
<th>MW (Exact)</th>
<th>MW (Experimental)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-Hydroxypropanoic acid</td>
<td>C3H6O3</td>
<td>90.0317</td>
<td>91.0395</td>
</tr>
<tr>
<td>3-Methyl-2-oxopentanoic acid</td>
<td>C6H10O3</td>
<td>130.0630</td>
<td>131.0708</td>
</tr>
<tr>
<td>4-Methyl-2-oxopentanoic acid</td>
<td>C6H10O3</td>
<td>130.0630</td>
<td>131.0708</td>
</tr>
<tr>
<td>4-Ethylheptanoic acid</td>
<td>C9H18O2</td>
<td>158.1307</td>
<td>159.1385</td>
</tr>
<tr>
<td>Phenylacetic acid</td>
<td>C8H8O2</td>
<td>136.0524</td>
<td>137.0603</td>
</tr>
<tr>
<td>4-Ethyldecanoic acid ('goat acid')</td>
<td>C10H20O2</td>
<td>172.1463</td>
<td>173.1542</td>
</tr>
<tr>
<td>Octanedioic acid (suberic acid)</td>
<td>C8H14O4</td>
<td>174.0892</td>
<td>175.097</td>
</tr>
<tr>
<td>9-Hydroxynonanoic acid</td>
<td>C9H18O3</td>
<td>174.1256</td>
<td>175.1334</td>
</tr>
<tr>
<td>(4-Hydroxyphenyl)acetic acid</td>
<td>C8H8O3</td>
<td>152.0473</td>
<td>153.0552</td>
</tr>
<tr>
<td>Nonanedioic acid (azelaic acid)</td>
<td>C9H16O4</td>
<td>188.1049</td>
<td>189.1127</td>
</tr>
<tr>
<td>2-ethylhexanoic acid</td>
<td>C8H16O2</td>
<td>144.115</td>
<td>145.1229</td>
</tr>
<tr>
<td>2-Piperidinone</td>
<td>C5H9NO</td>
<td>99.0684</td>
<td>100.0762</td>
</tr>
<tr>
<td>2-Methylhexanoic acid</td>
<td>C7H14O2</td>
<td>130.0994</td>
<td>131.1072</td>
</tr>
<tr>
<td>2-Methylheptanoic acid</td>
<td>C8H16O2</td>
<td>144.115</td>
<td>145.1229</td>
</tr>
<tr>
<td>2-Methyldecanoic acid</td>
<td>C9H18O2</td>
<td>158.1307</td>
<td>159.1385</td>
</tr>
</tbody>
</table>
2-Methylnonanoic acid

2-Methyldecanoic acid

8-Methylundecanoic acid

9-Methyldodecanoic acid

10-Methyltridecanoic acid

Isovaleric acid

3-Methylhexanoic acid

4-Ethylpentanoic acid

4-Ethylnonanoic acid

4-Ethyldecanoic acid

Propanoic acid

Hexanoic acid

Benzoic acid

Dodecanoic acid

Tetradecanoic acid

Pentadecanoic acid

Hexadecanoic acid

Heptadecanoic acid

2-Methylhexadecanoic acid

Octadecanoic acid
\begin{align*}
n\text{-Heptanoic acid} & \quad \text{C}_{7}\text{H}_{14}\text{O}_{2} & 130.0994 & 131.1072 \\
n\text{-Octanoic acid} & \quad \text{C}_{8}\text{H}_{16}\text{O}_{2} & 144.115 & 145.1229 \\
n\text{-Nonanoic acid} & \quad \text{C}_{9}\text{H}_{18}\text{O}_{2} & 158.1307 & 159.1385 \\
n\text{-Decanoic acid} & \quad \text{C}_{10}\text{H}_{20}\text{O}_{2} & 172.1463 & 173.1542 \\
n\text{-Undecanoic acid} & \quad \text{C}_{11}\text{H}_{22}\text{O}_{2} & 186.162 & 187.1698 \\
n\text{-Methyldodecanoic acid} & \quad \text{C}_{13}\text{H}_{26}\text{O}_{2} & 214.1933 & 215.2011 \\
-\text{Methyltetradecanoic acid} & \quad \text{C}_{15}\text{H}_{30}\text{O}_{2} & 242.2246 & 243.2324 \\
\text{Esters} & \ & \ & \\
7\text{-Hexadecenoic acid methyl ester} & \quad \text{C}_{17}\text{H}_{32}\text{O}_{2} & 268.2402 & 269.2481 \\
\text{Acetic acid phenylmethyl ester} & \quad \text{C}_{9}\text{H}_{10}\text{O}_{2} & 150.0681 & 151.0759 \\
2\text{-Phenylethyl acetate} & \quad \text{C}_{10}\text{H}_{12}\text{O}_{2} & 164.0837 & 165.0916 \\
\text{Cyclopentanetridecanoic acid methyl ester} & \quad \text{C}_{19}\text{H}_{36}\text{O}_{2} & 296.2715 & 297.2794 \\
\text{Dodecanoic acid, 10-methyl, methyl ester} & \quad \text{C}_{14}\text{H}_{28}\text{O}_{2} & 228.2089 & 229.2168 \\
\text{Furancarboxylic acid methyl ester} & \quad \text{C}_{6}\text{H}_{6}\text{O}_{3} & 126.0317 & 127.0395 \\
\text{Hexanedioic acid dimethyl ester} & \quad \text{C}_{8}\text{H}_{14}\text{O}_{4} & 174.0892 & 175.0970 \\
\text{Methyl 9-methyltetradecanoate} & \quad \text{C}_{16}\text{H}_{32}\text{O}_{2} & 256.2402 & 257.2481 \\
\text{Propanedioic acid dimethyl ester} & \quad \text{C}_{5}\text{H}_{8}\text{O}_{4} & 132.0423 & 133.0501 \\
\text{Hexanoic acid methyl ester} & \quad \text{C}_{7}\text{H}_{14}\text{O}_{2} & 130.0994 & 131.1072 \\
\text{Octanoic acid methyl ester} & \quad \text{C}_{9}\text{H}_{18}\text{O}_{2} & 158.1307 & 159.1385 \\
\text{Nonanoic acid methyl ester} & \quad \text{C}_{10}\text{H}_{20}\text{O}_{2} & 172.1463 & 173.1542 \\
\text{Decanoic acid methyl ester} & \quad \text{C}_{11}\text{H}_{22}\text{O}_{2} & 186.162 & 187.1698 \\
\end{align*}
Undecanoic acid methyl ester
\( \text{C}_{12}\text{H}_{24}\text{O}_2 \)
200.1776 201.1855

Dodecanoic acid methyl ester
\( \text{C}_{13}\text{H}_{26}\text{O}_2 \)
214.1933 215.2011

Tridecanoic acid methyl ester
\( \text{C}_{14}\text{H}_{28}\text{O}_2 \)
228.2089 229.2168

Tetradecanoic acid methyl ester
\( \text{C}_{15}\text{H}_{30}\text{O}_2 \)
242.2246 243.2324

Pentadecanoic acid methyl ester
\( \text{C}_{16}\text{H}_{32}\text{O}_2 \)
256.2402 257.2481

Hexadecanoic acid methyl ester
\( \text{C}_{17}\text{H}_{34}\text{O}_2 \)
270.2559 271.2637

Heptadecanoic acid methyl ester
\( \text{C}_{18}\text{H}_{36}\text{O}_2 \)
284.2715 285.2794

9-Hexadecenoic acid methyl ester
\( \text{C}_{17}\text{H}_{32}\text{O}_2 \)
268.2402 269.2481

Terpinyl acetate
\( \text{C}_{12}\text{H}_{20}\text{O}_2 \)
196.1463 197.1542

Methyl-N'-methylanthranilate
\( \text{C}_{9}\text{H}_{11}\text{NO}_2 \)
165.079 166.0868

2-Hexyl 2-pentenoate
\( \text{C}_{11}\text{H}_{20}\text{O}_2 \)
184.1463 185.1542

E-Cinnamyl acetate
\( \text{C}_{11}\text{H}_{12}\text{O}_2 \)
176.0837 177.0916

α-Trichloromethyl-benzyl acetate
\( \text{C}_{10}\text{H}_{9}\text{Cl}_3\text{O}_2 \)
265.9668 266.9746

Isoeugenol acetate
\( \text{C}_{12}\text{H}_{14}\text{O}_3 \)
206.0943 207.1021

Dihydromyrcenol acetate
\( \text{C}_{12}\text{H}_{20}\text{O}_2 \)
196.1463 197.1542

Neryl acetate
\( \text{C}_{12}\text{H}_{20}\text{O}_2 \)
196.1463 197.1542

Geranyl acetate
\( \text{C}_{12}\text{H}_{20}\text{O}_2 \)
196.1463 197.1542

Citronellol acetate
\( \text{C}_{12}\text{H}_{22}\text{O}_2 \)
198.162 199.1698

Methylcis-dihydrojasmonate
\( \text{C}_{12}\text{H}_{19}\text{O}_3 \)
211.1334 212.1412
Pentyl salicylate

Methyl trans-jasmonate

1-Hexenyl salicylate

1-Hexyl salicylate

2-Ethylhexyl salicylate

Ethyl tetradecanoate

Ethyl pentadecanoate

Ethyl hexadecanoate

Benzyl benzoate

2-phenylethyl phenylacetate

Isopropyl dodecanoate

Dodecyl hexanoate

Hexadecanoic acid isopropyl ester

Ethyl heptadecanoate

Dodecyl benzoate

Tridecyl benzoate

Tetradecyl benzoate
Decyl octanoate

Dodecyl octanoate

Tetradecyl octanoate

2-Ethylhexyl 4-methoxycinnamate

1-Octyl 4-methoxycinnamate

2-Ethyl-hexyl 4-methoxycinnamate

Isooctanedioldibutyrate

Amines

2-Pentylpyrrole

2-Phenoxyethylmethylamine

Nicotine

4-Sec-butylaniline

N,N-Dimethyl-1-dodecylamine

N,N-Dimethyl-1-hexadecylamine

N,N-Dimethyl-1-octadecylamine

Amides

Methyl N,N-dimethylthiocarbamate

n-Propylbenzamide

Hydroxy acetanilide

Aldehydes

2-Furancarboxaldehyde

Benzaldehyde
<table>
<thead>
<tr>
<th>Compound</th>
<th>Structural Formula</th>
<th>Molecular Formula</th>
<th>Exact Mass (m/z)</th>
<th>Retention Time (min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hexanal</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O} )</td>
<td>100.0888, 101.0966</td>
<td></td>
</tr>
<tr>
<td>Heptanal</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>7\text{H}</em>{14}\text{O} )</td>
<td>114.1045, 115.1123</td>
<td></td>
</tr>
<tr>
<td>Octanal</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>8\text{H}</em>{16}\text{O} )</td>
<td>128.1201, 129.1279</td>
<td></td>
</tr>
<tr>
<td>Nonanal</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>9\text{H}</em>{18}\text{O} )</td>
<td>142.1358, 143.1436</td>
<td></td>
</tr>
<tr>
<td>Decanal</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>{10}\text{H}</em>{20}\text{O} )</td>
<td>156.1514, 157.1592</td>
<td></td>
</tr>
<tr>
<td>Undecanal</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>{11}\text{H}</em>{22}\text{O} )</td>
<td>170.1671, 171.1749</td>
<td></td>
</tr>
<tr>
<td>Dodecanal</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>{12}\text{H}</em>{24}\text{O} )</td>
<td>184.1827, 185.1905</td>
<td></td>
</tr>
<tr>
<td>Tridecanal</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>{13}\text{H}</em>{26}\text{O} )</td>
<td>198.1984, 199.2062</td>
<td></td>
</tr>
<tr>
<td>Tetradecanal</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>{14}\text{H}</em>{28}\text{O} )</td>
<td>212.214, 213.2218</td>
<td></td>
</tr>
<tr>
<td>Hexadecanal</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>{16}\text{H}</em>{32}\text{O} )</td>
<td>240.2453, 241.2531</td>
<td></td>
</tr>
<tr>
<td>(E)-2-Nonenal</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>9\text{H}</em>{16}\text{O} )</td>
<td>140.1201, 141.1279</td>
<td></td>
</tr>
<tr>
<td>Geranial</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>{10}\text{H}</em>{16}\text{O} )</td>
<td>152.1201, 153.1279</td>
<td></td>
</tr>
<tr>
<td>p-Anisaldehyde</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}_8\text{H}_8\text{O}_2 )</td>
<td>136.0524, 137.0524</td>
<td></td>
</tr>
<tr>
<td>Pentylcinnamaldehyde</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>{14}\text{H}</em>{18}\text{O} )</td>
<td>202.1358, 203.1436</td>
<td></td>
</tr>
<tr>
<td>E-2-Hexylcinnamaldehyde</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>{15}\text{H}</em>{20}\text{O} )</td>
<td>216.1514, 217.1592</td>
<td></td>
</tr>
</tbody>
</table>

**Ketones**

<table>
<thead>
<tr>
<th>Compound</th>
<th>Structural Formula</th>
<th>Molecular Formula</th>
<th>Exact Mass (m/z)</th>
<th>Retention Time (min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6,10-Dimethyl-5,9-undecadien-2-one</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>{13}\text{H}</em>{22}\text{O} )</td>
<td>194.1671, 195.1749</td>
<td></td>
</tr>
<tr>
<td>6-Methyl-5-hepten-2-one</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>8\text{H}</em>{14}\text{O} )</td>
<td>126.1045, 127.1123</td>
<td></td>
</tr>
<tr>
<td>α-Ionone</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>{13}\text{H}</em>{20}\text{O} )</td>
<td>192.1514, 193.1592</td>
<td></td>
</tr>
<tr>
<td>β-Ionone</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>{13}\text{H}</em>{20}\text{O} )</td>
<td>192.1514, 193.1592</td>
<td></td>
</tr>
<tr>
<td>Benzophenone</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>{13}\text{H}</em>{10}\text{O} )</td>
<td>182.0732, 183.0810</td>
<td></td>
</tr>
<tr>
<td>Jasmone</td>
<td>( \text{CH}_3 \text{CO} )</td>
<td>( \text{C}<em>{11}\text{H}</em>{16}\text{O} )</td>
<td>164.1201, 165.1279</td>
<td></td>
</tr>
</tbody>
</table>
Acetophenone

Isopropylacetophenone

2-Nonanone

2-Undecanone

2-Dodecanone

2-Tridecanone

2-Tetradecanone

2-Pentadecanone

2-Hexadecanone

Alcohols

Tridecan-1-ol

n-Tetradecanol

Pentadecanol

n-Hexadecanol

a Hexadecadienol

2-Furanmethanol

Phenol

Benzyl Alcohol

2-Phenylethanol

p-Menth-1-en-8-ol

Geraniol

Citronellol

Eugenol
<table>
<thead>
<tr>
<th>Compound</th>
<th>Molecular Formula</th>
<th>Mass</th>
<th>Molecular Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isoeugenol</td>
<td>C10H12O2</td>
<td>164.0837</td>
<td>165.0916</td>
</tr>
<tr>
<td>2-Phenoxyethanol</td>
<td>C8H10O2</td>
<td>138.0681</td>
<td>139.0759</td>
</tr>
<tr>
<td><strong>Aliphatic/Aromatic</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nonane</td>
<td>C9H20</td>
<td>128.1565</td>
<td>129.1643</td>
</tr>
<tr>
<td>Undecane</td>
<td>C11H24</td>
<td>156.1878</td>
<td>157.1956</td>
</tr>
<tr>
<td>Dodecane</td>
<td>C12H26</td>
<td>170.2035</td>
<td>171.2113</td>
</tr>
<tr>
<td>Tridecane</td>
<td>C13H28</td>
<td>184.2191</td>
<td>185.2269</td>
</tr>
<tr>
<td>Tetradecane</td>
<td>C14H30</td>
<td>198.2348</td>
<td>199.2426</td>
</tr>
<tr>
<td>Pentadecane</td>
<td>C15H32</td>
<td>212.2504</td>
<td>213.2582</td>
</tr>
<tr>
<td>Hexadecane</td>
<td>C16H34</td>
<td>226.2661</td>
<td>227.2739</td>
</tr>
<tr>
<td>Heptadecane</td>
<td>C17H36</td>
<td>240.2817</td>
<td>241.2895</td>
</tr>
<tr>
<td>Octadecane</td>
<td>C18H38</td>
<td>254.2974</td>
<td>255.3052</td>
</tr>
<tr>
<td>Nonadecane</td>
<td>C19H40</td>
<td>268.3130</td>
<td>269.3208</td>
</tr>
<tr>
<td>Eicosane</td>
<td>C20H42</td>
<td>282.3287</td>
<td>283.3365</td>
</tr>
<tr>
<td>Heneicosane</td>
<td>C21H44</td>
<td>296.3443</td>
<td>297.3521</td>
</tr>
<tr>
<td>Docosane</td>
<td>C22H46</td>
<td>310.3600</td>
<td>311.3678</td>
</tr>
<tr>
<td>Tricosane</td>
<td>C23H48</td>
<td>324.3756</td>
<td>325.3834</td>
</tr>
<tr>
<td>Tetracosane</td>
<td>C24H50</td>
<td>338.3913</td>
<td>339.3991</td>
</tr>
<tr>
<td>3-Methylloctadecane</td>
<td>C19H40</td>
<td>268.3130</td>
<td>269.3208</td>
</tr>
<tr>
<td>3-Methylnonadecane</td>
<td>C20H42</td>
<td>282.3287</td>
<td>283.3365</td>
</tr>
<tr>
<td>4-Methylpentadecane</td>
<td>C16H34</td>
<td>226.2661</td>
<td>227.2739</td>
</tr>
<tr>
<td>Nonane, 1-chloro-</td>
<td>ClC9H19</td>
<td>162.1175</td>
<td>163.1254</td>
</tr>
</tbody>
</table>
| Pyridine                 | ClS5H5N           | 79.0422 | 80.0500
<table>
<thead>
<tr>
<th>Name</th>
<th>Molecular Formula</th>
<th>Exact Mass (m/z) 1</th>
<th>Exact Mass (m/z) 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>α-Pinene</td>
<td>C10H16</td>
<td>136.1252</td>
<td>137.1330</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>C10H8</td>
<td>128.0626</td>
<td>129.0704</td>
</tr>
<tr>
<td>Cyclotetradecane</td>
<td>C14H28</td>
<td>196.2191</td>
<td>197.2269</td>
</tr>
<tr>
<td>Toluene</td>
<td>C7H8</td>
<td>92.0626</td>
<td>93.0704</td>
</tr>
<tr>
<td>p-Cymene</td>
<td>C10H14</td>
<td>134.1096</td>
<td>135.1174</td>
</tr>
<tr>
<td>Methyl biphenyl</td>
<td>C13H12</td>
<td>168.0939</td>
<td>169.1017</td>
</tr>
<tr>
<td>2-Phenylandecane</td>
<td>C17H28</td>
<td>232.2191</td>
<td>233.2269</td>
</tr>
<tr>
<td>3-Phenylandecane</td>
<td>C17H28</td>
<td>232.2191</td>
<td>233.2269</td>
</tr>
<tr>
<td>4-Phenylandecane</td>
<td>C17H28</td>
<td>232.2191</td>
<td>233.2269</td>
</tr>
<tr>
<td>5-Phenylandecane</td>
<td>C17H28</td>
<td>232.2191</td>
<td>233.2269</td>
</tr>
<tr>
<td>6-Phenylandecane</td>
<td>C17H28</td>
<td>232.2191</td>
<td>233.2269</td>
</tr>
<tr>
<td>2-Phenyldodecane</td>
<td>C18H30</td>
<td>246.2348</td>
<td>247.2426</td>
</tr>
<tr>
<td>5-Phenyldodecane</td>
<td>C18H30</td>
<td>246.2348</td>
<td>247.2426</td>
</tr>
<tr>
<td>6-Phenyldodecane</td>
<td>C18H30</td>
<td>246.2348</td>
<td>247.2426</td>
</tr>
<tr>
<td>2-Phenyltridecane</td>
<td>C19H32</td>
<td>260.2504</td>
<td>261.2582</td>
</tr>
<tr>
<td>3-Phenyltridecane</td>
<td>C19H32</td>
<td>260.2504</td>
<td>261.2582</td>
</tr>
<tr>
<td>4-Phenyltridecane</td>
<td>C19H32</td>
<td>260.2504</td>
<td>261.2582</td>
</tr>
<tr>
<td>6-Phenyltridecane</td>
<td>C19H32</td>
<td>260.2504</td>
<td>261.2582</td>
</tr>
<tr>
<td>1-Dodecene</td>
<td>C12H24</td>
<td>168.1878</td>
<td>169.1956</td>
</tr>
<tr>
<td>1-Tetradecene</td>
<td>C14H28</td>
<td>196.2191</td>
<td>197.2269</td>
</tr>
<tr>
<td>1-Nonadecene</td>
<td>C19H38</td>
<td>266.2974</td>
<td>267.3052</td>
</tr>
<tr>
<td>Farnesene</td>
<td>C15H24</td>
<td>204.1878</td>
<td>205.1956</td>
</tr>
</tbody>
</table>
### Precursors

- N-α-3-methylhex-2-enoyl-L-glutamine
  - C\textsubscript{12}H\textsubscript{20}N\textsubscript{2}O\textsubscript{4}
  - 256.1423 \text {Da}
  - 257.1501 \text {Da}

- N-α-3-hydroxy-3-methylhexanoyl- L-glutamine
  - C\textsubscript{12}H\textsubscript{22}N\textsubscript{2}O\textsubscript{5}
  - 274.1529 \text {Da}
  - 275.1607 \text {Da}

- S-[1-(2-hydroxy-1-methylethyl)-2-methylethyl]-L-cysteineylglycine
  - C\textsubscript{11}H\textsubscript{22}N\textsubscript{2}O\textsubscript{4}S
  - 278.1300 \text {Da}
  - 279.1379 \text {Da}

- S-[1-(2-hydroxy-1-methylethyl)-1-ethyl]-L-cysteine
  - C\textsubscript{8}H\textsubscript{17}NO\textsubscript{3}S
  - 207.0929 \text {Da}
  - 208.1007 \text {Da}

- S-[1-(2-hydroxyethyl)-1-methylbutyl]-L-cysteinylglycine
  - C\textsubscript{12}H\textsubscript{24}N\textsubscript{2}O\textsubscript{4}S
  - 292.1457 \text {Da}
  - 293.1535 \text {Da}

- N-α-3-hydroxy-4-methylheptanoyl- L-glutamine
  - C\textsubscript{13}H\textsubscript{24}N\textsubscript{2}O\textsubscript{4}
  - 284.1736 \text {Da}
  - 285.1814 \text {Da}

- N-α-3-methyl-2-oxopentanoyl- L-glutamine
  - C\textsubscript{11}H\textsubscript{18}N\textsubscript{2}O\textsubscript{5}
  - 258.1216 \text {Da}
  - 259.1294 \text {Da}

- N-α-3-methyl-2-oxopentanoyl- L-glutamine
  - C\textsubscript{11}H\textsubscript{18}N\textsubscript{2}O\textsubscript{5}
  - 258.1216 \text {Da}
  - 259.1294 \text {Da}

- N-α-3-methyl-2-oxopentanoyl- L-glutamine
  - C\textsubscript{11}H\textsubscript{18}N\textsubscript{2}O\textsubscript{5}
  - 258.1216 \text {Da}
  - 259.1294 \text {Da}
N-α-4-ethyl-hept-anoyl- L-glutamine

N-α-4-hydroxyphenyl-acetyl- L-glutamine

N-α-4-ethyl-oct-anoyl- L-glutamine

N-α-7-carboxy-hept-anoyl- L-glutamine

N-α-9-hydroxy- non-anoyl- L-glutamine

Hypothetical Precursors

N-α-3-hydroxy- 3-methylhept-anoyl- L-glutamine

N-α-3-hydroxy-oct-anoyl- L-glutamine

N-α-8-hydroxy-oct-anoyl- L-glutamine

TCA Cycle Intermediates

Citrate

Aconitate

Isocitrate

α-Ketoglutarate

Succinate

Fumarate
<table>
<thead>
<tr>
<th>Compound</th>
<th>Molecular Formula</th>
<th>Mass (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Malate</td>
<td>C₄H₄O₅⁻²</td>
<td>132.0059</td>
</tr>
<tr>
<td></td>
<td></td>
<td>133.0137</td>
</tr>
<tr>
<td>Oxaloacetate</td>
<td>C₄H₂O₅⁻²</td>
<td>129.9902</td>
</tr>
<tr>
<td></td>
<td></td>
<td>130.9980</td>
</tr>
<tr>
<td>Pyruvic acid</td>
<td>C₃H₄O₃</td>
<td>88.0160</td>
</tr>
<tr>
<td></td>
<td></td>
<td>89.0238</td>
</tr>
</tbody>
</table>