

# Supplementary Materials: Gas Chromatography–Mass Spectrometry Profiling of Volatile Compounds Reveals Metabolic Changes in a Non-Aflatoxigenic *Aspergillus flavus* Induced by 5-Azacytidine

Fengqin Song, Qingru Geng, Xuewei Wang, Xiaoqing Gao, Xiaona He, Wei Zhao, Huahui Lan, Jun Tian, Kunlong Yang and Shihua Wang

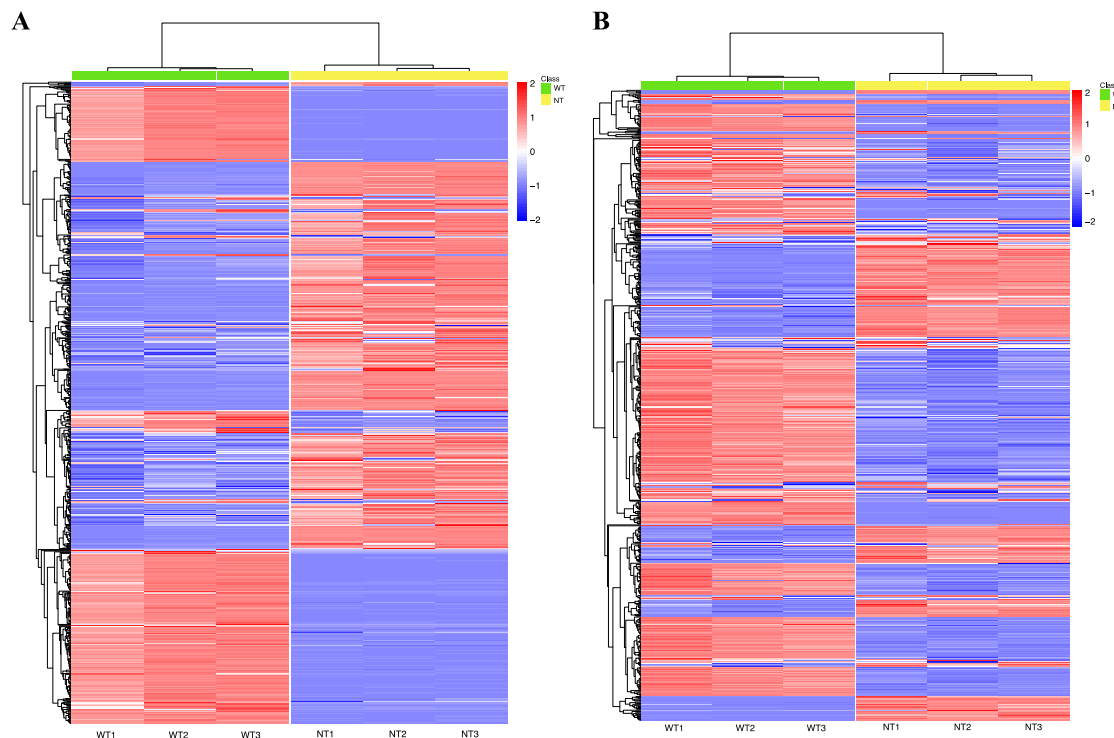
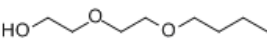
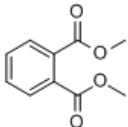
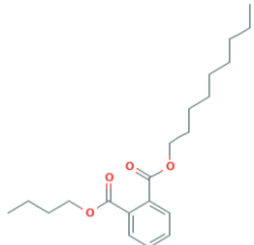
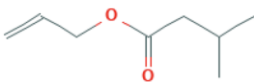
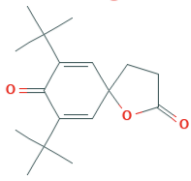
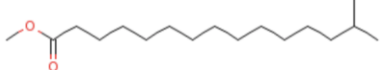
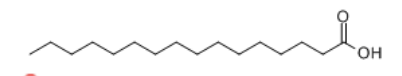
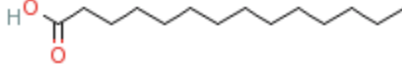
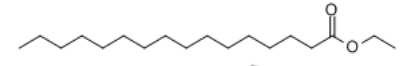
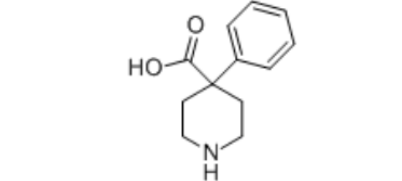
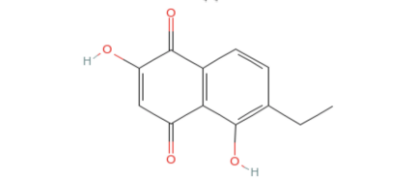
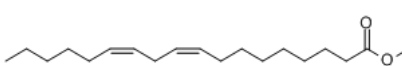
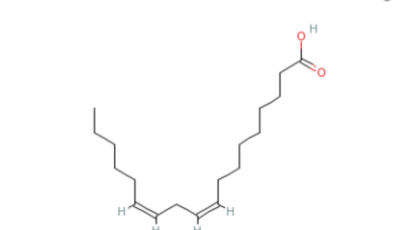
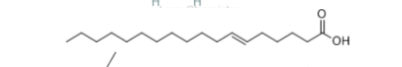
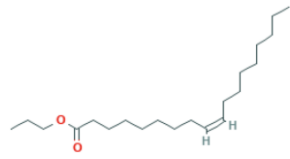
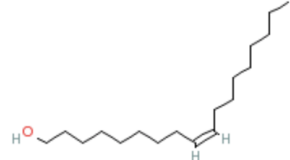
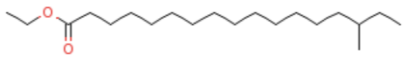
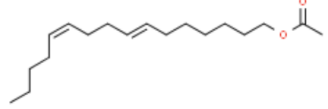
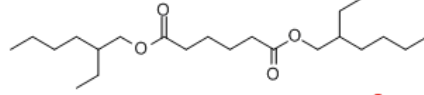
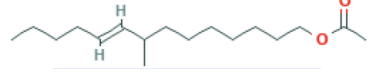
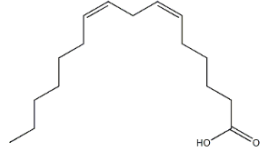


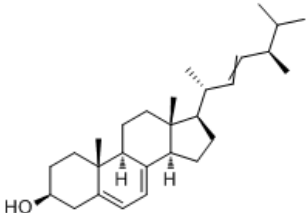
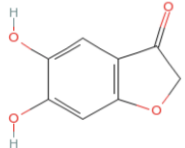
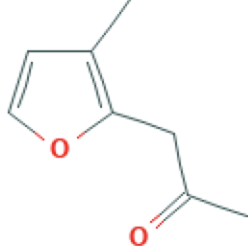
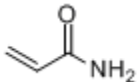
**Figure S1.** Clustering and heatmap visualization of the identified volatile metabolites in WT and NT strains both in vitro and in vivo. **(A)** Clustering and heatmap visualization of the identified volatile metabolites in WT (A133 strain) and NT strains in vitro. **(B)** Clustering and heatmap visualization of the identified volatile metabolites in WT and NT strains in vivo.

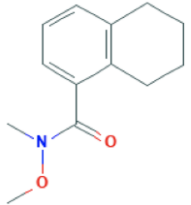
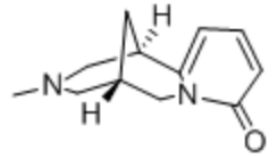
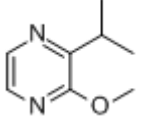
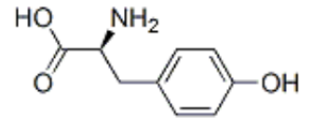
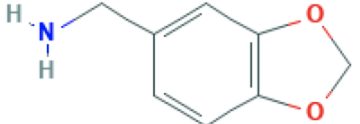
**Table S1.** Volatile metabolites assessed via GC-MS analysis in WT (A133 strain) and NT strains in vitro were analyzed with the Agilent ChemStation software. The chemical structure or the chemical structural formula was analyzed in pubchem database (<https://pubchem.ncbi.nlm.nih.gov>).

| RT (min)                            | Compound Name                                             | Quality (%) | mz      | CAS Number  | Structure                                                                             | Formula                                        | WT | NT |
|-------------------------------------|-----------------------------------------------------------|-------------|---------|-------------|---------------------------------------------------------------------------------------|------------------------------------------------|----|----|
| <b>Fatty Acid Derived Volatiles</b> |                                                           |             |         |             |                                                                                       |                                                |    |    |
| 19.361                              | Ethanol,2-(2-butoxyethoxy)-                               | 90          | 162.126 | 000112-34-5 |    | C <sub>8</sub> H <sub>18</sub> O <sub>3</sub>  | Y  | Y  |
| 28.330                              | Dimethylphthalate                                         | 91          | 194.058 | 000131-11-3 |    | C <sub>10</sub> H <sub>10</sub> O <sub>4</sub> | Y  | Y  |
| 39.928                              | Phthalicacid,isobutylonylester                            | 90          | 348.23  | 003461-31-2 |    | C <sub>21</sub> H <sub>32</sub> O <sub>4</sub> | Y  | N  |
| 40.499                              | Allyl isovalerate                                         | 30          | 142.099 | 002833-93-4 |   | C <sub>8</sub> H <sub>14</sub> O <sub>2</sub>  | Y  | N  |
| 41.000                              | 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione | 99          | 276.173 | 082304-66-3 |  | C <sub>17</sub> H <sub>24</sub> O <sub>3</sub> | Y  | Y  |
| 41.700                              | Pentadecanoicacid,14-methyl-,methylester                  | 74          | 270.256 | 005129-60-2 |  | C <sub>17</sub> H <sub>34</sub> O <sub>2</sub> | Y  | Y  |

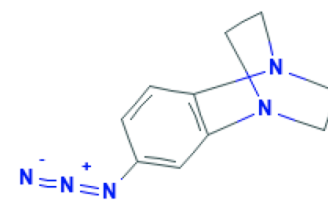
|        |                                                |    |         |              |                                                                                       |                                                     |   |   |
|--------|------------------------------------------------|----|---------|--------------|---------------------------------------------------------------------------------------|-----------------------------------------------------|---|---|
| 42.542 | n-Hexadecanoic acid                            | 93 | 256.24  | 000057-10-3  |    | C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>      | Y | N |
| 42.996 | Tetradecanoic acid                             | 93 | 228.209 | 000544-63-8  |    | C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>      | Y | N |
| 43.325 | Hexadecanoic acid, ethylester                  | 98 | 284.272 | 000628-97-7  |    | C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>      | Y | N |
| 44.343 | Normeperidinic acid                            | 59 | 205     | 003627-45-0  |    | C <sub>12</sub> H <sub>15</sub> N<br>O <sub>2</sub> | Y | Y |
| 45.441 | 1,4-Naphthoquinone, 6-ethyl-2,5-dihydroxy-     | 38 | 218.058 | 013378-87-5  |    | C <sub>12</sub> H <sub>10</sub> O <sub>4</sub>      | Y | N |
| 45.600 | 9,12-Octadecadienoic acid (Z,Z)-, methyl ester | 99 | 294.256 | 000112-63-0  |    | C <sub>19</sub> H <sub>34</sub> O <sub>2</sub>      | Y | N |
| 46.496 | 9,12-Octadecadienoic acid (Z,Z)-               | 99 | 280.24  | 000060-33-3  |   | C <sub>18</sub> H <sub>32</sub> O <sub>2</sub>      | Y | N |
| 46.628 | 6-Octadecenoic acid                            | 96 | 282.256 | 1000336-66-8 |  | C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>      | Y | N |
| 47.111 | 9,12-Octadecadienoic acid, ethylester          | 99 | 308.272 | 007619-08-1  |  | C <sub>20</sub> H <sub>36</sub> O <sub>2</sub>      | Y | N |

|        |                                         |    |         |              |                                                                                      |                                                |   |   |
|--------|-----------------------------------------|----|---------|--------------|--------------------------------------------------------------------------------------|------------------------------------------------|---|---|
| 47.272 | n-Propyl9-octadecenoate                 | 64 | 324.303 | 1000336-71-6 |   | C <sub>21</sub> H <sub>40</sub> O <sub>2</sub> | Y | N |
| 47.660 | OleylAlcohol                            | 90 | 268.277 | 000143-28-2  |   | C <sub>18</sub> H <sub>36</sub> O              | Y | N |
| 47.894 | Heptadecanoicacid,15-methyl-,ethylester | 94 | 312.303 | 057274-46-1  |   | C <sub>20</sub> H <sub>40</sub> O <sub>2</sub> | Y | N |
| 51.116 | Z,E-7,11-Hexadecadien-1-yl acetate      | 51 | 280.24  | 051607-94-4  |   | C <sub>18</sub> H <sub>32</sub> O <sub>2</sub> | N | Y |
| 51.951 | Hexanedioicacid,bis(2-ethylhexyl)ester  | 93 | 370.308 | 000103-23-1  |   | C <sub>22</sub> H <sub>42</sub> O <sub>4</sub> | Y | N |
| 52.434 | E-8-Methyl-9-tetradecen-1-ol acetate    | 38 | 268.24  | 1000130-81-4 |   | C <sub>17</sub> H <sub>32</sub> O <sub>2</sub> | Y | N |
| 60.276 | 6,9-hexadecadienoic acid                | 55 | 252.39  | 1000253-06-3 |  | C <sub>16</sub> H <sub>28</sub> O <sub>2</sub> | Y | N |

|                                      |                                              |    |         |             |                                                                                       |                                               |   |   |
|--------------------------------------|----------------------------------------------|----|---------|-------------|---------------------------------------------------------------------------------------|-----------------------------------------------|---|---|
| 66.434                               | Ergosterol                                   | 94 | 396.339 | 000057-87-4 |    | C <sub>28</sub> H <sub>44</sub> O             | Y | N |
| <b>Saccharide Derived Volatiles</b>  |                                              |    |         |             |                                                                                       |                                               |   |   |
| 34.400                               | Benzo[b]tetrahydrofuran-3-one,5,6-dihydroxy- | 59 | 166.027 | 014771-00-7 |    | C <sub>8</sub> H <sub>6</sub> O <sub>4</sub>  | Y | Y |
| 53.474                               | 3-Methyl-2-(2-oxopropyl)furan                | 49 | 138.068 | 087773-62-4 |    | C <sub>8</sub> H <sub>10</sub> O <sub>2</sub> | Y | N |
| <b>Amino Acids Derived Volatiles</b> |                                              |    |         |             |                                                                                       |                                               |   |   |
| 6.203                                | 2-Propenamide                                | 72 | 71.037  | 000079-06-1 |  | C <sub>3</sub> H <sub>5</sub> NO              | N | Y |

|        |                                                     |    |         |             |                                                                                      |                    |   |   |
|--------|-----------------------------------------------------|----|---------|-------------|--------------------------------------------------------------------------------------|--------------------|---|---|
| 29.333 | N-Methyl-N-methoxy-5,6,7,8-tetrahydro-1-naphthamide | 64 | 219.126 | 185957-97-5 |   | $C_{13}H_{17}NO_2$ | Y | N |
| 29.700 | Caulophylline                                       | 86 | 204.27  | 000486-86-2 |   | $C_{12}H_{16}N_2O$ | Y | Y |
| 31.903 | Pyrazine,2-methoxy-3-(1-methylethyl)-               | 49 | 152.095 | 025773-40-4 |   | $C_8H_{12}N_2O$    | N | Y |
| 33.200 | L-Tyrosine                                          | 94 | 182     | 000060-18-4 |   | $C_9H_9NO_3$       | Y | Y |
| 33.206 | Piperonylamine                                      | 38 | 151.063 | 002620-50-0 |  | $C_8H_9NO_2$       | N | Y |

33.895 4'-Azidobenzo[1',2'-b]-  
1,4-  
diazabicyclo[2.2.2]octe  
ne 25 201.101 120287-75-4

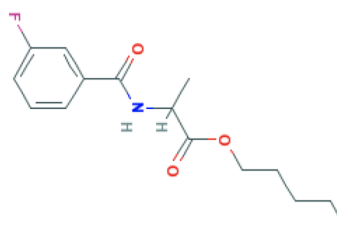


C<sub>10</sub>H<sub>11</sub>N<sub>5</sub>

Y

N

34.927 l-Alanine,N-(3-  
fluorobenzoyl)-  
,pentylester 64 281.143 1000314-20-8

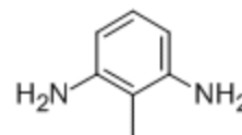


C<sub>15</sub>H<sub>20</sub>F  
NO<sub>3</sub>

Y

N

35.022 2,6-toluenediamine 59 122.17 000823-40-5

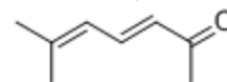


C<sub>7</sub>H<sub>10</sub>N<sub>2</sub>

N

Y

35.930 6-Methyl-3,5-  
heptadien-2-one 91 124.18 001921-70-6

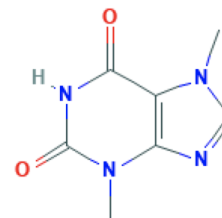


C<sub>8</sub>H<sub>12</sub>O

N

Y

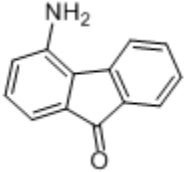
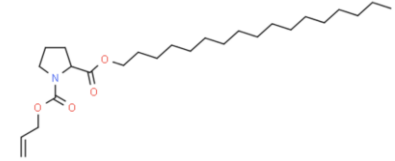
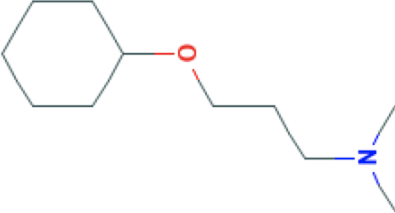
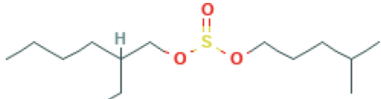
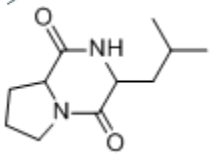
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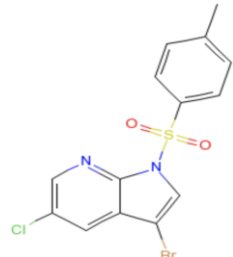
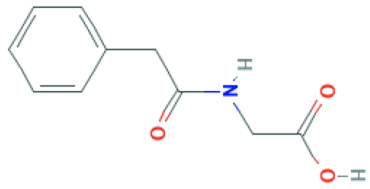
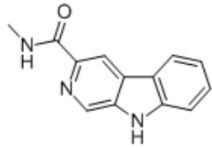
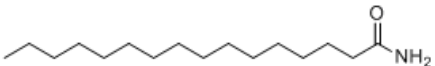
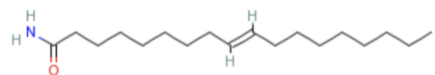
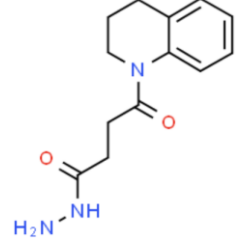


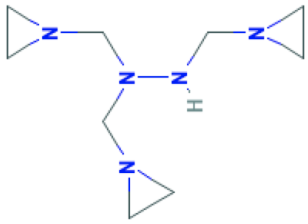
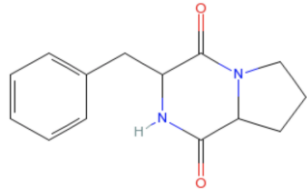
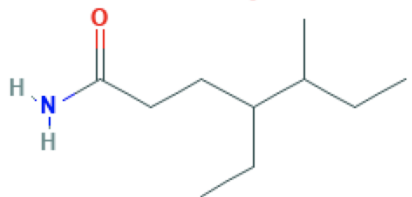
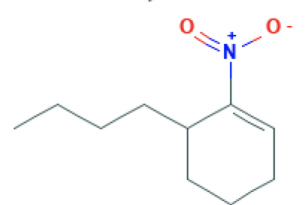
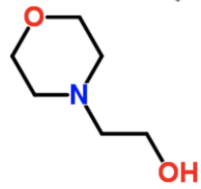
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O<sub>2</sub>

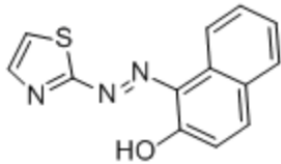
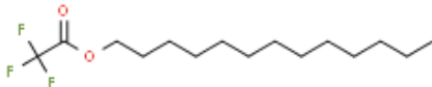
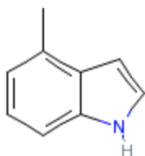
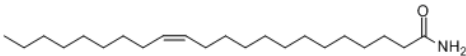
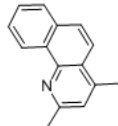
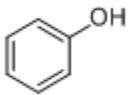
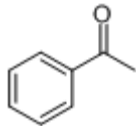
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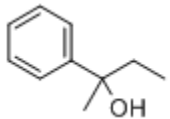
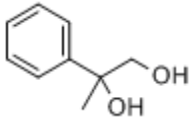
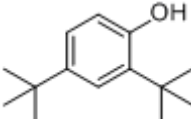
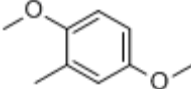
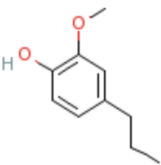
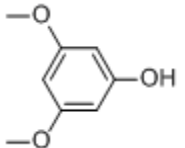
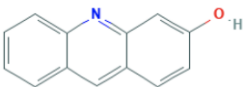
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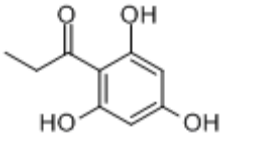
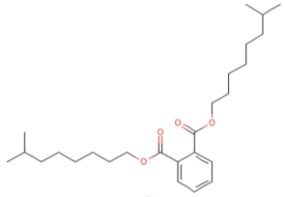
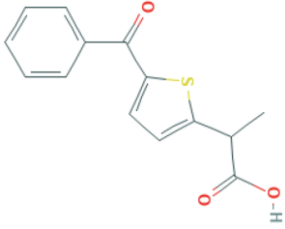
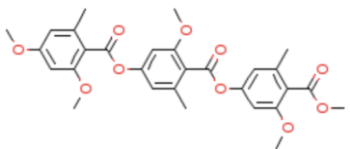
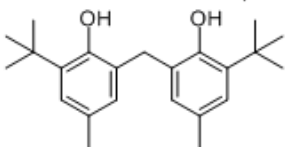
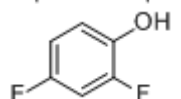
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| 38.317 | 4-Amino-9-fluorenone                                            | 46 | 195.068 | 004269-15-2  |   | $C_{13}H_9NO$        | Y | N |
| 41.019 | d-Proline, N-allyloxycarbonyl-, heptadecyl ester                | 43 | 437.351 | 1000320-97-6 |   | $C_{26}H_{47}NO_4$   | N | Y |
| 41.180 | 3-Cyclohexyloxypropylamine, N,N-dimethyl-                       | 50 | 185.178 | 071126-67-5  |   | $C_{11}H_{23}NO$     | N | Y |
| 41.253 | Sulfurous acid, 2-ethylhexyl isohexyl ester                     | 38 | 278.192 | 1000309-19-0 |   | $C_{27}H_{56}$       | Y | Y |
| 41.480 | Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)- | 64 | 210.137 | 005654-86-4  |  | $C_{11}H_{18}N_2O_2$ | N | Y |

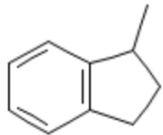
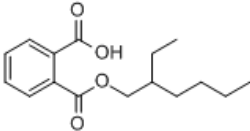
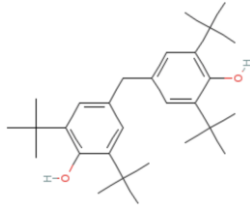
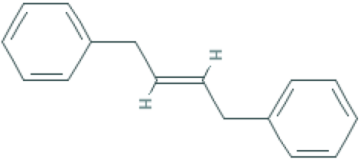
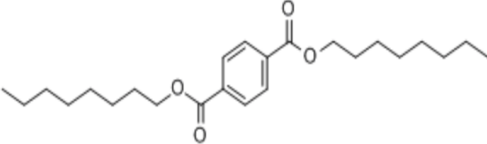
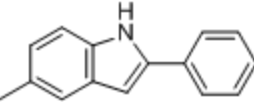
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|--------|---------------------------------------------------------------|----|---------|-------------|---------------------------------------------------------------------------------------|---------------------------------|---|---|
| 41.500 | Diethyldithiophosphinic acid                                  | 38 | 154.004 | 000866-54-6 |    | $C_{14}H_{10}Br$<br>$ClN_2O_2S$ | Y | Y |
| 41.663 | Phenylacetylglycine                                           | 27 | 193.202 | 000500-98-1 |    | $C_{10}H_{11}N$<br>$O_3$        | N | Y |
| 46.210 | N-Methyl-beta-carboline-3-carboxamide                         | 94 | 225.25  | 078538-74-6 |    | $C_{13}H_{11}N_3$<br>$O$        | N | Y |
| 47.418 | Hexadecanamide                                                | 97 | 255.256 | 000629-54-9 |    | $C_{16}H_{33}N$<br>$O$          | N | Y |
| 47.455 | 9-Octadecenamide,(Z)-                                         | 95 | 281.272 | 000301-02-0 |   | $C_{18}H_{35}N$<br>$O$          | Y | N |
| 49.747 | 4-(3,4-Dihydro-2H-quinolin-1-yl)-4-oxo-butyric acid hydrazide | 43 | 247.132 | 315673-61-1 |  | $C_{13}H_{17}N_3$<br>$O_2$      | Y | N |

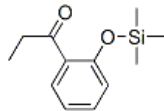
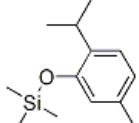
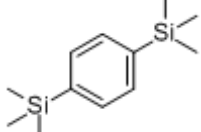
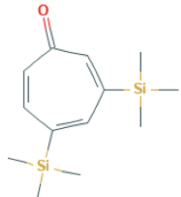
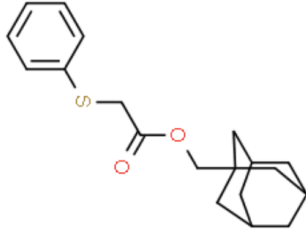
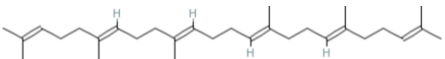
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|--------|---------------------------------------------------------------|----|---------|--------------|---------------------------------------------------------------------------------------|----------------------|---|---|
| 50.040 | Tris(aziridinomethyl)hydrazine                                | 58 | 197.164 | 1000254-64-1 |    | $C_{34}H_{70}$       | Y | N |
| 50.413 | Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(phenylmethyl)- | 49 | 244.121 | 014705-60-3  |    | $C_{14}H_{16}N_2O_2$ | N | Y |
| 51.270 | Heptanamide, 4-ethyl-5-methyl-                                | 42 | 171.162 | 054789-40-1  |    | $C_{10}H_{21}NO$     | Y | Y |
| 53.298 | Cyclohexene, 6-butyl-1-nitro-                                 | 46 | 183.126 | 084820-13-3  |   | $C_{10}H_{17}NO_2$   | Y | N |
| 54.404 | 4-Morpholineethanol                                           | 46 | 131.095 | 000622-40-2  |  | $C_6H_{13}NO_2$      | Y | N |

|                                               |                                       |    |         |             |                                                                                       |                                                     |   |   |
|-----------------------------------------------|---------------------------------------|----|---------|-------------|---------------------------------------------------------------------------------------|-----------------------------------------------------|---|---|
| 54.887                                        | 1-(2-Thiazolylazo)-2-naphthol         | 81 | 255.5   | 001147-56-4 |    | C <sub>13</sub> H <sub>9</sub> N <sub>3</sub><br>OS | Y | N |
| 55.487                                        | Trifluoroacetic acid,n-tridecyl ester | 38 | 296.196 | 053800-02-5 |    | C <sub>15</sub> H <sub>27</sub> F                   | Y | N |
| 57.450                                        | 1H-Indole,4-methyl-                   | 43 | 131.073 | 016096-32-5 |    | C <sub>9</sub> H <sub>9</sub> N                     | Y | N |
| 59.177                                        | 13-Docosenamide,(Z)-                  | 35 | 337.334 | 000112-84-5 |    | C <sub>22</sub> H <sub>43</sub> N<br>O              | Y | N |
| 66.741                                        | Benzo[h]quinoline,2,4-dimethyl-       | 45 | 207.105 | 000605-67-4 |    | C <sub>15</sub> H <sub>13</sub> N                   | Y | N |
| <b>Phenylpropanoid Derivatives/Benzenoids</b> |                                       |    |         |             |                                                                                       |                                                     |   |   |
| 10.977                                        | Phenol                                | 25 | 94.042  | 000108-95-2 |   | C <sub>6</sub> H <sub>6</sub> O                     | N | Y |
| 14.506                                        | Acetophenone                          | 91 | 120.058 | 000098-86-2 |  | C <sub>8</sub> H <sub>8</sub> O                     | Y | Y |

|        |                                           |    |         |             |                                                                                       |                                                |   |   |
|--------|-------------------------------------------|----|---------|-------------|---------------------------------------------------------------------------------------|------------------------------------------------|---|---|
| 15.399 | .alpha.-Ethyl-.alpha.-methylbenzylalcohol | 72 | 150.104 | 001565-75-9 |    | C <sub>10</sub> H <sub>14</sub> O              | N | Y |
| 15.400 | dl-2-Phenyl-1,2-propanediol               | 78 | 152.084 | 004217-66-7 |    | 152.19                                         | Y | Y |
| 30.182 | Phenol,2,4-bis(1,1-dimethylethyl)-        | 96 | 206.167 | 000096-76-4 |    | C <sub>14</sub> H <sub>22</sub> O              | Y | Y |
| 31.793 | Benzene,1,4-dimethoxy-2-methyl-           | 70 | 152.084 | 024599-58-4 |    | C <sub>9</sub> H <sub>12</sub> O <sub>2</sub>  | Y | N |
| 34.429 | Phenol,2-methoxy-4-propyl-                | 59 | 166.099 | 002785-87-7 |    | C <sub>10</sub> H <sub>14</sub> O <sub>2</sub> | N | Y |
| 38.581 | Phenol,3,5-dimethoxy-                     | 47 | 154.063 | 000500-99-2 |   | C <sub>8</sub> H <sub>10</sub> O <sub>3</sub>  | N | Y |
| 38.317 | 3-Acridinol                               | 43 | 195.068 | 007132-70-9 |  | C <sub>13</sub> H <sub>9</sub> N<br>O          | Y | Y |

|        |                                                                            |    |         |              |                                                                                       |                                                     |   |   |
|--------|----------------------------------------------------------------------------|----|---------|--------------|---------------------------------------------------------------------------------------|-----------------------------------------------------|---|---|
| 38.600 | Flopropione                                                                | 38 | 182.058 | 002295-58-1  |    | C <sub>9</sub> H <sub>10</sub> O <sub>4</sub>       | Y | Y |
| 42.293 | Phthalicacid,bis(7-methyloctyl)ester                                       | 59 | 418.308 | 020548-62-3  |    | C <sub>26</sub> H <sub>42</sub> O <sub>4</sub>      | N | Y |
| 49.754 | Tiaprofenic acid                                                           | 43 | 260.31  | 1000227-01-4 |    | C <sub>14</sub> H <sub>12</sub> O <sub>3</sub><br>S | N | Y |
| 50.516 | 4,2-Cresoticacid,6-methoxy-,bimol.ester,methylester,4,6-dimethoxy-otoluate | 47 | 538.184 | 019314-74-0  |   | C <sub>29</sub> H <sub>30</sub> O <sub>10</sub>     | N | Y |
| 52.207 | Phenol,2,2'-methylenebis[6-(1,1-dimethylethyl)-4-methyl-                   | 95 | 340.24  | 000119-47-1  |  | C <sub>23</sub> H <sub>32</sub> O <sub>2</sub>      | Y | Y |
| 53.642 | 2,4-Difluorophenol                                                         | 35 | 130.023 | 000367-27-1  |  | C <sub>6</sub> H <sub>4</sub> F <sub>2</sub> O      | Y | N |

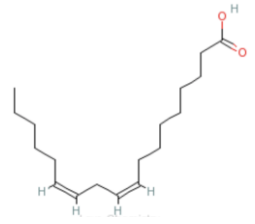
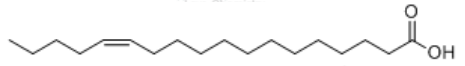
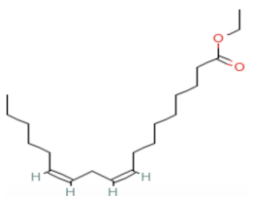
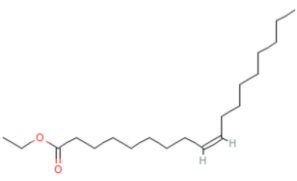
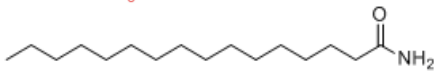
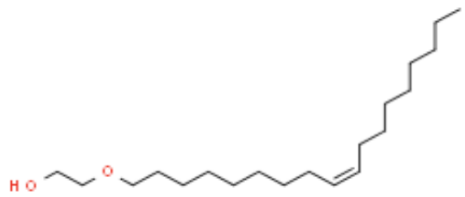
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|--------|--------------------------------------------------------|----|---------|--------------|---------------------------------------------------------------------------------------|------------------------------------------------|---|---|
| 54.015 | Indan,1-methyl-                                        | 47 | 132.094 | 000767-58-8  |    | C <sub>10</sub> H <sub>12</sub>                | Y | N |
| 54.674 | 1,2-Benzenedicarboxylic acid, mono(2-ethylhexyl) ester | 90 | 278.152 | 004376-20-9  |    | C <sub>16</sub> H <sub>22</sub> O <sub>4</sub> | Y | Y |
| 55.172 | Phenol,4,4'-methylenebis[2,6-bis(1,1-dimethylethyl)-   | 55 | 424.334 | 000118-82-1  |    | C <sub>29</sub> H <sub>44</sub> O <sub>2</sub> | N | Y |
| 57.757 | Benzene,1,1'-(2-butene-1,4-diyl)bis-                   | 45 | 208.125 | 013657-49-3  |    | C <sub>16</sub> H <sub>16</sub>                | Y | N |
| 58.555 | Terephthalic acid, di(2-ethylhexyl) ester              | 46 | 390.277 | 1000324-01-0 |   | C <sub>24</sub> H <sub>38</sub> O <sub>4</sub> | Y | N |
| 59.404 | 1H-Indole,5-methyl-2-phenyl-                           | 18 | 207.105 | 013228-36-9  |  | C <sub>15</sub> H <sub>13</sub> N              | Y | N |

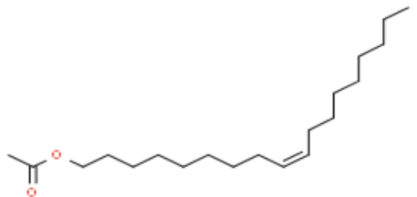
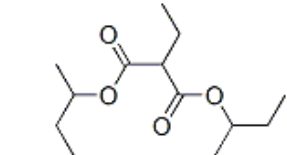
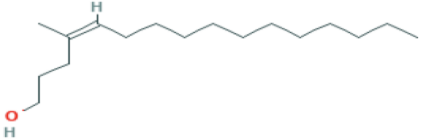
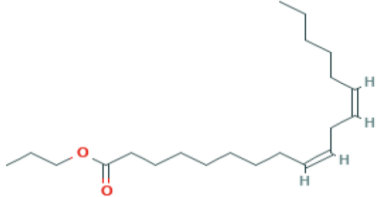
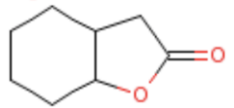
|                   |                                                                       |    |         |              |                                                                                       |                                                      |   |   |
|-------------------|-----------------------------------------------------------------------|----|---------|--------------|---------------------------------------------------------------------------------------|------------------------------------------------------|---|---|
| 62.004            | Propiophenone,2'-(trimethylsiloxy)-                                   | 38 | 222.108 | 033342-87-9  |    | C <sub>12</sub> H <sub>18</sub> O <sub>2</sub><br>Si | Y | N |
| 62.590            | Silane,trimethyl[5-methyl-2-(1-methylethyl)phenoxy]                   | 49 | 222.144 | 055012-80-1  |    | C <sub>13</sub> H <sub>22</sub> O<br>Si              | Y | N |
| 65.592            | Silane,1,4-phenylenebis(trimethyl-)                                   | 53 | 222.126 | 013183-70-5  |    | C <sub>12</sub> H <sub>22</sub> Si <sub>2</sub>      | Y | N |
| 65.767            | 2,4,6-Cycloheptatrien-1-one,3,5-bis-trimethylsilyl-                   | 50 | 250.121 | 1000161-21-8 |    | C <sub>13</sub> H <sub>22</sub> O<br>Si <sub>2</sub> | Y | N |
| 66.880            | (Phenylthio)acetic acid, 1-adamantylmethyl ester                      | 25 | 316.15  | 1000299-95-7 |   | C <sub>19</sub> H <sub>24</sub> O <sub>2</sub><br>S  | N | Y |
| <b>Triterpene</b> |                                                                       |    |         |              |                                                                                       |                                                      |   |   |
| 59.851            | 2,6,10,14,18,22-Tetracosahexaene,2,6,10,15,19,23-hexamethyl-,(all-E)- | 99 | 410.391 | 000111-02-4  |  | C <sub>30</sub> H <sub>50</sub>                      | Y | N |

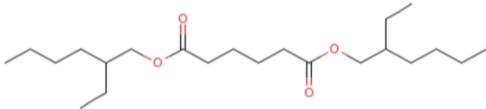
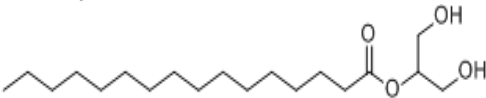
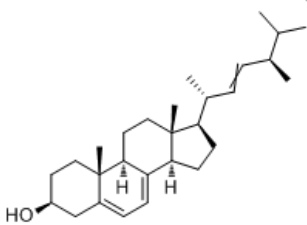
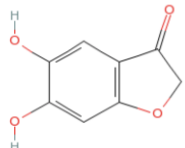
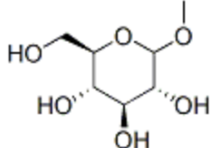
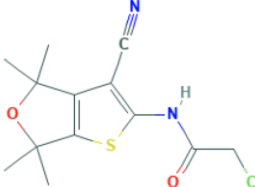
‘Y’ indicates the compound identified in the strain, ‘N’ indicates that the compound is not detected in the strain.

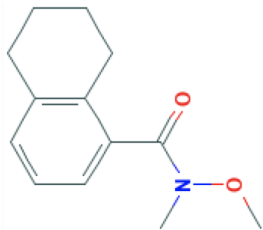
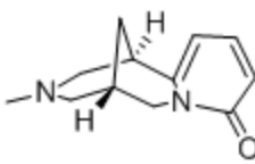
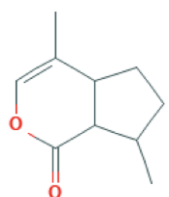
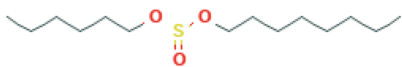
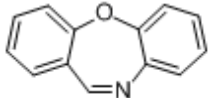
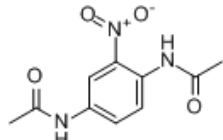
**Table S2.** Volatile metabolites assessed via GC-MS analysis in WT (A133 strain) and NT strains *in vivo* were analyzed with the Agilent ChemStation software. The chemical structure or the chemical structural formula was analyzed in pubchem database (<https://pubchem.ncbi.nlm.nih.gov>).

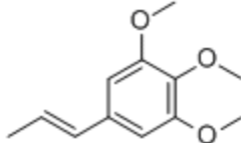
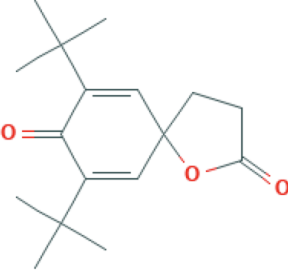
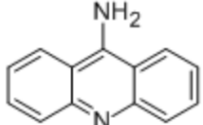
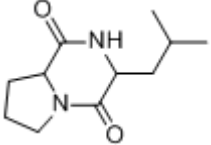
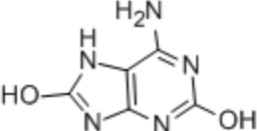
| RT (min)                            | Volatile Compound                                       | Quality (%) | mz      | CAS Number   | Structure | Chemical Structural Formula                      | WT | NT |
|-------------------------------------|---------------------------------------------------------|-------------|---------|--------------|-----------|--------------------------------------------------|----|----|
| <b>Fatty Acid Derived Volatiles</b> |                                                         |             |         |              |           |                                                  |    |    |
| 19.361                              | Ethanol,2-(2-butoxyethoxy)-                             | 90          | 162.126 | 000112-34-5  |           | C <sub>8</sub> H <sub>18</sub> O <sub>3</sub>    | Y  | Y  |
| 31.046                              | Sulfurous acid, isohexyl pentyl ester                   | 50          | 236.145 | 1000309-14-0 |           | C <sub>11</sub> H <sub>24</sub> O <sub>3</sub> S | Y  | N  |
| 39.935                              | 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester | 78          | 278.152 | 000084-69-5  |           | C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>   | Y  | N  |
| 41.663                              | Hexadecanoic acid, methyl ester                         | 95          | 270.256 | 000112-39-0  |           | C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>   | Y  | Y  |
| 42.491                              | n-Hexadecanoic acid                                     | 99          | 256.24  | 000057-10-3  |           | C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>   | Y  | Y  |
| 43.318                              | Hexadecanoic acid, ethyl ester                          | 96          | 284.272 | 000628-97-7  |           | C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>   | Y  | Y  |

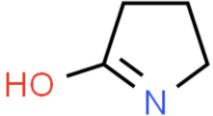
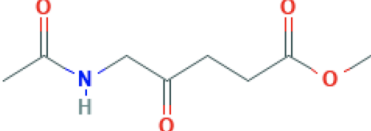
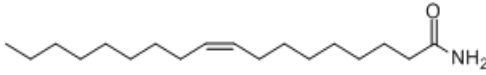
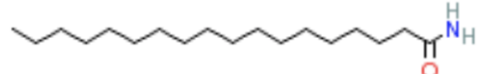
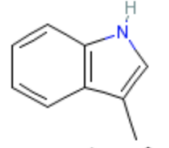
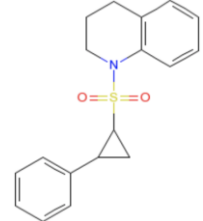
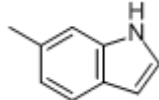
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|--------|-------------------------------------|----|---------|-------------|---------------------------------------------------------------------------------------|------------------------------------------------|---|---|
| 46.43  | 9,12-Octadecadienoic acid (Z,Z)-    | 99 | 280.24  | 000060-33-3 |    | C <sub>18</sub> H <sub>32</sub> O <sub>2</sub> | Y | Y |
| 46.576 | cis-13-Octadecenoic acid            | 98 | 282.256 | 013126-39-1 |    | C <sub>18</sub> H <sub>34</sub> O <sub>2</sub> | Y | Y |
| 47.111 | Linoleic acid diethyl ester         | 99 | 308.272 | 000544-35-4 |    | C <sub>20</sub> H <sub>36</sub> O <sub>2</sub> | Y | Y |
| 47.265 | Ethyl Oleate                        | 99 | 310.287 | 000111-62-6 |    | C <sub>20</sub> H <sub>38</sub> O <sub>2</sub> | Y | Y |
| 47.433 | Hexadecanamide                      | 99 | 255.256 | 000629-54-9 |   | C <sub>16</sub> H <sub>33</sub> NO             | N | Y |
| 47.645 | Ethanol, 2-(9-octadecenyoxy)-, (Z)- | 70 | 312.303 | 005353-25-3 |  | C <sub>20</sub> H <sub>38</sub>                | Y | N |

|        |                                                      |    |         |              |                                                                                       |                                                |   |   |
|--------|------------------------------------------------------|----|---------|--------------|---------------------------------------------------------------------------------------|------------------------------------------------|---|---|
| 47.66  | Oleyl alcohol , acetate                              | 60 | 310.287 | 1000352-67-9 |    | C <sub>20</sub> H <sub>38</sub>                | N | Y |
| 47.894 | Octadecanoic acid, ethyl ester                       | 95 | 312.303 | 000111-61-5  |    | C <sub>20</sub> H <sub>40</sub> O <sub>2</sub> | N | Y |
| 49.754 | Propanedioic acid, ethyl-, bis(1-methylpropyl) ester | 47 | 244.167 | 057983-52-5  |    | C <sub>13</sub> H <sub>24</sub> O <sub>4</sub> | N | Y |
| 50.728 | 4-Methyl-Z-4-hexadecen-1-ol                          | 38 | 254.261 | 1000130-89-0 |    | C <sub>17</sub> H <sub>34</sub> O              | Y | Y |
| 51.116 | n-Propyl 9,12-octadecadienoate                       | 49 | 322.287 | 1000336-77-8 |   | C <sub>21</sub> H <sub>38</sub> O <sub>2</sub> | N | Y |
| 51.116 | cis-7-Oxabicyclo[4.3.0]nonan-8-one                   | 47 | 140.084 | 024871-12-3  |  | C <sub>8</sub> H <sub>12</sub> O <sub>2</sub>  | Y | Y |

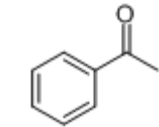
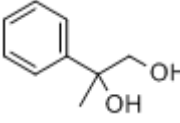
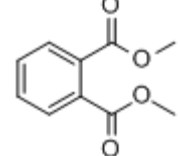
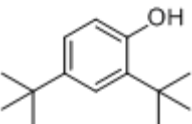
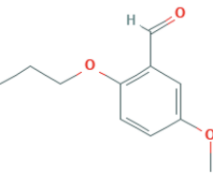
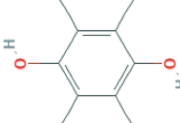
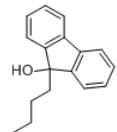
|                                     |                                                                                        |    |         |              |                                                                                       |                                                                   |   |   |
|-------------------------------------|----------------------------------------------------------------------------------------|----|---------|--------------|---------------------------------------------------------------------------------------|-------------------------------------------------------------------|---|---|
| 51.951                              | Hexanedioicacid,bis(2-ethylhexyl)ester                                                 | 93 | 370.308 | 000103-23-1  |    | C <sub>22</sub> H <sub>42</sub> O <sub>4</sub>                    | Y | Y |
| 54.411                              | Hexadecanoicacid,2-hydroxy-1-(hydroxymethyl)ethylester                                 | 43 | 330.277 | 023470-00-0  |    | C <sub>19</sub> H <sub>38</sub> O <sub>4</sub>                    | Y | N |
| 66.448                              | Ergosterol                                                                             | 74 | 396.339 | 000057-87-4  |    | C <sub>28</sub> H <sub>44</sub> O                                 | Y | Y |
| <b>Saccharide Derived Volatiles</b> |                                                                                        |    |         |              |                                                                                       |                                                                   |   |   |
| 34.781                              | Benzo[b]tetrahydrofuran-3-one,5,6-dihydroxy-                                           | 59 | 166.027 | 014771-00-7  |    | C <sub>8</sub> H <sub>6</sub> O <sub>4</sub>                      | Y | Y |
| 41.253                              | D-Glucoside                                                                            | 50 | 194.18  | 000097-30-3  |   | C <sub>7</sub> H <sub>14</sub> O <sub>6</sub>                     | Y | Y |
| 66.873                              | Acetamide,2-chloro-N-(3-cyano-4,6-dihydro-4,4,6,6-tetramethylthieno[2,3-c]furan-2-yl)- | 4  | 298.054 | 1000350-39-4 |  | C <sub>13</sub> H <sub>15</sub> ClN <sub>2</sub> O <sub>2</sub> S | Y | N |

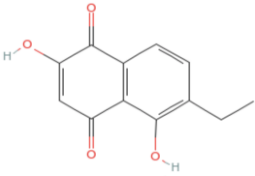
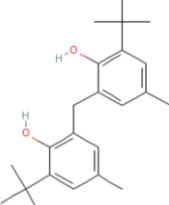
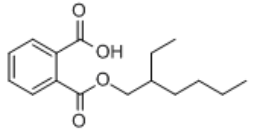
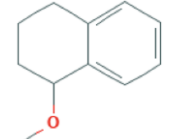
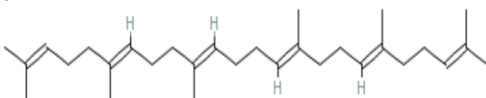
| Amino Acids Derived Volatiles |                                                     |    |         |              |                                                                                       |                                                               |   |   |
|-------------------------------|-----------------------------------------------------|----|---------|--------------|---------------------------------------------------------------------------------------|---------------------------------------------------------------|---|---|
| 29.333                        | N-Methyl-N-methoxy-5,6,7,8-tetrahydro-1-naphthamide | 64 | 219.126 | 185957-97-5  |    | C <sub>13</sub> H <sub>17</sub> NO <sub>2</sub>               | Y | N |
| 29.655                        | Caulophylline                                       | 87 | 204.27  | 000486-86-2  |    | C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O              | Y | N |
| 34.986                        | Nepetalactone                                       | 46 | 166.099 | 000490-10-8  |    | C <sub>10</sub> H <sub>14</sub> O <sub>2</sub>                | Y | N |
| 35.784                        | Sulfurous acid, hexyl octyl ester                   | 53 | 278.192 | 1000309-13-0 |   | C <sub>14</sub> H <sub>30</sub> O <sub>3</sub> S              | N | Y |
| 38.31                         | Dibenz[b,f][1,4]oxazepine                           | 43 | 195.068 | 000257-07-8  |  | C <sub>13</sub> H <sub>9</sub> NO                             | Y | N |
| 38.617                        | N,N'-Diacetyl-2-nitro-p-phenylenediamine            | 53 | 237.075 | 005345-53-9  |  | C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O <sub>4</sub> | Y | N |

|        |                                                                |    |         |              |                                                                                       |                                                               |   |   |
|--------|----------------------------------------------------------------|----|---------|--------------|---------------------------------------------------------------------------------------|---------------------------------------------------------------|---|---|
| 40.111 | Isoelemicin                                                    | 64 | 208.25  | 1000323-76-1 |    | C <sub>12</sub> H <sub>16</sub> O <sub>3</sub>                | N | Y |
| 41.004 | 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione      | 99 | 276.173 | 082304-66-3  |    | C <sub>17</sub> H <sub>24</sub> O <sub>3</sub>                | Y | Y |
| 41.202 | 9-Aminoacridine                                                | 50 | 194.23  | 097825-91-7  |    | C <sub>13</sub> H <sub>10</sub> N <sub>2</sub>                | N | Y |
| 41.473 | Pyrrolo[1,2-a]pyrazine-1,4-dione,hexahydro-3-(2-methylpropyl)- | 53 | 210.137 | 005654-86-4  |   | C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub> | Y | N |
| 42.3   | 2,8-Dihydroxyadenine                                           | 58 | 167.12  | 30377-37-8   |  | C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O <sub>2</sub>   | Y | Y |

|        |                                                                        |    |         |             |                                                                                       |                                                      |   |   |
|--------|------------------------------------------------------------------------|----|---------|-------------|---------------------------------------------------------------------------------------|------------------------------------------------------|---|---|
| 46.21  | 2-Pyrrolidinone                                                        | 18 | 85.053  | 000616-45-5 |    | C <sub>5</sub> H <sub>5</sub> O <sub>2</sub>         | Y | N |
| 49.754 | Pentanoic acid, 5-(acetylamino)-4-oxo-, methyl ester                   | 43 | 187.084 | 093393-93-2 |    | C <sub>8</sub> H <sub>13</sub> NO <sub>4</sub>       | Y | Y |
| 51.277 | 9-Octadecenamide,(Z)-                                                  | 99 | 281.272 | 000301-02-0 |    | C <sub>18</sub> H <sub>35</sub> NO                   | Y | Y |
| 51.826 | Octadecanamide                                                         | 94 | 283.288 | 000124-26-5 |    | C <sub>18</sub> H <sub>37</sub> NO                   | Y | Y |
| 53.642 | 1H-Indole,3-methyl-                                                    | 47 | 131.073 | 000083-34-1 |    | C <sub>9</sub> H <sub>9</sub> N                      | Y | Y |
| 54.037 | Quinoline,1,2,3,4-tetrahydro-1-((2-phenylcyclopropyl)sulfonyl)-,trans- | 43 | 313.114 | 017299-24-0 |   | C <sub>18</sub> H <sub>19</sub> NO <sub>2</sub><br>S | N | Y |
| 57.449 | 1H-Indole, 6-methyl-                                                   | 43 | 131.073 | 003420-02-8 |  | C <sub>9</sub> H <sub>9</sub> N                      | N | Y |

## Phenylpropanoid Derivatives/Benzenoids

|        |                                    |    |         |              |                                                                                       |                                                |   |   |
|--------|------------------------------------|----|---------|--------------|---------------------------------------------------------------------------------------|------------------------------------------------|---|---|
| 14.506 | Acetophenone                       | 91 | 120.058 | 000098-86-2  |    | C <sub>8</sub> H <sub>8</sub> O                | Y | Y |
| 15.400 | dl-2-Phenyl-1,2-propanediol        | 78 | 152.084 | 004217-66-7  |    | 152.19                                         | Y | Y |
| 28.330 | Dimethylphthalate                  | 91 | 194.058 | 000131-11-3  |    | C <sub>10</sub> H <sub>10</sub> O <sub>4</sub> | Y | Y |
| 30.182 | Phenol,2,4-bis(1,1-dimethylethyl)- | 96 | 206.167 | 000096-76-4  |    | C <sub>14</sub> H <sub>22</sub> O              | Y | Y |
| 31.91  | Benzaldehyde,-2-propoxy,-5-methoxy | 60 | 194.094 | 1000222-96-5 |   | C <sub>11</sub> H <sub>14</sub> O <sub>3</sub> | N | Y |
| 35.22  | Durohydroquinone                   | 72 | 166.099 | 000527-18-4  |  | C <sub>10</sub> H <sub>14</sub> O <sub>2</sub> | N | Y |
| 44.307 | 9H-Fluoren-9-ol,9-butyl-           | 56 | 238.136 | 005806-10-0  |  | C <sub>17</sub> H <sub>18</sub> O              | N | Y |

|            |                                                                        |    |         |             |                                                                                       |                                                |   |   |
|------------|------------------------------------------------------------------------|----|---------|-------------|---------------------------------------------------------------------------------------|------------------------------------------------|---|---|
| 45.441     | 1,4-Naphthoquinone,6-ethyl-2,5-dihydroxy-                              | 25 | 218.058 | 013378-87-5 |    | C <sub>12</sub> H <sub>10</sub> O <sub>4</sub> | Y | N |
| 52.207     | Phenol,2,2'-methylenebis[6-(1,1-dimethylethyl)-4-methyl-               | 94 | 340.24  | 000119-47-1 |    | C <sub>23</sub> H <sub>32</sub> O <sub>2</sub> | Y | Y |
| 54.674     | 1,2-Benzenedicarboxylic acid, mono(2-ethylhexyl)ester                  | 91 | 278.152 | 004376-20-9 |    | C <sub>16</sub> H <sub>22</sub> O <sub>4</sub> | Y | Y |
| 57.449     | Naphthalene,1,2,3,4-tetrahydro-1-methoxy-                              | 43 | 162.104 | 001008-18-0 |    | C <sub>11</sub> H <sub>14</sub> O              | Y | Y |
| Triterpene |                                                                        |    |         |             |                                                                                       |                                                |   |   |
| 59.851     | 2,6,10,14,18,22-Tetracosahexaene,2,6,10,15,19,23-hexamethyl-, (all-E)- | 99 | 410.391 | 000111-02-4 |  | C <sub>30</sub> H <sub>50</sub>                | Y | Y |

'Y' indicates the compound identified in the strain, 'N' indicates that the compound is not detected in the strain.