**Table S1. The result of the aroma profile evaluation**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| tea samples | Score of each aroma attribute | | | | | | | |
| chestnut-like | fresh | floral | fruity | sweety | fermented aroma | roasty | burning |
| NO.1 | 8 | 9 | 6 | 3 | 2 | 0 | 1 | 0 |
| NO.2 | 5 | 9 | 8 | 3 | 1 | 0 | 2 | 0 |
| NO.3 | 3 | 9 | 3 | 0 | 0 | 0 | 1 | 0 |
| NO.4 | 6 | 9 | 5 | 2 | 0 | 0 | 3 | 0 |
| NO.5 | 3 | 9 | 4 | 0 | 0 | 0 | 1 | 0 |
| NO.6 | 5 | 9 | 6 | 1 | 0 | 0 | 2 | 0 |
| NO.7 | 7 | 8 | 7 | 1 | 2 | 0 | 5 | 0 |
| NO.8 | 5 | 9 | 5 | 1 | 1 | 0 | 4 | 0 |
| NO.9 | 3 | 9 | 6 | 0 | 0 | 0 | 2 | 0 |
| NO.10 | 1 | 5 | 9 | 9 | 7 | 4 | 8 | 0 |
| NO.11 | 1 | 6 | 9 | 7 | 6 | 3 | 6 | 0 |
| NO.12 | 1 | 8 | 9 | 6 | 5 | 3 | 5 | 0 |
| NO.13 | 1 | 8 | 9 | 6 | 6 | 3 | 7 | 0 |
| NO.14 | 1 | 5 | 9 | 8 | 7 | 4 | 8 | 0 |
| NO.15 | 0 | 3 | 7 | 7 | 9 | 5 | 5 | 0 |
| NO.16 | 0 | 3 | 8 | 7 | 9 | 4 | 5 | 0 |
| NO.17 | 0 | 1 | 8 | 6 | 9 | 6 | 6 | 0 |
| NO.18 | 0 | 0 | 3 | 5 | 8 | 5 | 7 | 8 |

**Table S2. the qualitative results of 18 kinds of teas by HS-GC-IMS**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Count | Compounds1 | Formula | MW | RI2 | Rt [sec]3 | Dt [RIPrel]4 |
| 1 | propionaldehyde | C3H6O | 58.1 | 815 | 244.408 | 1.1459 |
| 2 | acetone | C3H6O | 58.1 | 836 | 253.842 | 1.1168 |
| 3 | acrolein | C3H4O | 56.1 | 872 | 271.695 | 1.062 |
| 4 | ethyl acetate | C4H8O2 | 88.1 | 902 | 288.81 | 1.3394 |
| 5 | 2,5-dimethylfuran | C6H8O | 96.1 | 911 | 294.418 | 1.0274 |
| 6 | 2-butanone | C4H8O | 72.1 | 916 | 297.569 | 1.2471 |
| 7 | 3-methylbutanal | C5H10O | 86.1 | 930 | 307.349 | 1.402 |
| 8 | ethanol | C2H6O | 46.1 | 946 | 318.006 | 1.0415 |
| 9 | 2-ethylfuran | C6H8O | 96.1 | 962 | 330.116 | 1.0469 |
| 10 | 2,3-butanedione | C4H6O2 | 86.1 | 974 | 340.028 | 1.165 |
| 11 | pentanal | C5H10O | 86.1 | 992 | 354.88 | 1.4258 |
| 12 | ethyl acrylate | C5H8O2 | 100.1 | 1017 | 377.782 | 1.1265 |
| 13 | 2,3-pentanedione | C5H8O2 | 100.1 | 1018 | 379.62 | 1.2238 |
| 14 | ethyl 2-methylbutanoate | C7H14O2 | 130.2 | 1019 | 380.585 | 1.2333 |
| 15 | ethyl 3-methylbutanoate | C7H14O2 | 130.2 | 1023 | 383.726 | 1.2567 |
| 16 | propyl acetate M | C5H10O2 | 102.1 | 1025 | 386.176 | 1.1654 |
| 17 | propyl acetate D | C5H10O2 | 102.1 | 1026 | 387.166 | 1.4781 |
| 18 | ethyl propanoate | C5H10O2 | 102.1 | 1027 | 387.763 | 1.145 |
| 19 | α-pinene | C10H16 | 136.2 | 1027 | 388.409 | 1.2163 |
| 20 | 1-propanol | C3H8O | 60.1 | 1040 | 401.381 | 1.1083 |
| 21 | ethyl butanoate M | C6H12O2 | 116.2 | 1048 | 409.833 | 1.2061 |
| 22 | ethyl butanoate D | C6H12O2 | 116.2 | 1047 | 409.264 | 1.5602 |
| 23 | hexanal | C6H12O | 100.2 | 1093 | 463.902 | 1.5647 |
| 24 | 2-methylpropanol | C4H10O | 74.1 | 1102 | 475.837 | 1.1674 |
| 25 | β-pinene | C10H16 | 136.2 | 1111 | 488.409 | 1.2191 |
| 26 | butyl propionate | C7H14O2 | 130.2 | 1134 | 523.595 | 1.2806 |
| 27 | butanol M | C4H10O | 74.1 | 1157 | 559.819 | 1.1835 |
| 28 | butanol D | C4H10O | 74.1 | 1157 | 560.347 | 1.3788 |
| 29 | 2-methylbutanol | C5H12O | 88.1 | 1170 | 584.007 | 1.2328 |
| 30 | pentyl acetate | C7H14O2 | 130.2 | 1188 | 617.101 | 1.3121 |
| 31 | ethyl valerate | C7H14O2 | 130.2 | 1192 | 623.905 | 1.2635 |
| 32 | 2-heptanone | C7H14O | 114.2 | 1197 | 633.374 | 1.6304 |
| 33 | heptanal | C7H14O | 114.2 | 1204 | 648.026 | 1.3284 |
| 34 | limonene M | C10H16 | 136.2 | 1208 | 657.706 | 1.2196 |
| 35 | limonene D | C10H16 | 136.2 | 1209 | 658.563 | 1.291 |
| 36 | limonene T | C10H16 | 136.2 | 1208 | 657.283 | 1.656 |
| 37 | 3-methylbutanol M | C5H12O | 88.1 | 1223 | 688.846 | 1.243 |
| 38 | 3-methylbutanol D | C5H12O | 88.1 | 1222 | 687.023 | 1.4888 |
| 39 | o-xylene | C8H10 | 106.2 | 1226 | 694.721 | 1.0662 |
| 40 | ethyl caproate | C8H16O2 | 144.2 | 1233 | 712.352 | 1.3403 |
| 41 | 2-pentylfuran | C9H14O | 138.2 | 1246 | 742.491 | 1.2526 |
| 42 | 2-hexanol | C6H14O | 102.2 | 1248 | 746.443 | 1.2807 |
| 43 | cyclohexanone | C6H10O | 98.1 | 1259 | 774.362 | 1.1493 |
| 44 | beta-ocimene | C10H16 | 136.2 | 1262 | 783.593 | 1.2147 |
| 45 | 1-pentanol M | C5H12O | 88.1 | 1266 | 793.463 | 1.2526 |
| 46 | 1-pentanol D | C5H12O | 88.1 | 1267 | 794.98 | 1.5089 |
| 47 | (Z)-3-hexenyl acetate | C8H14O2 | 142.2 | 1268 | 799.496 | 1.3039 |
| 48 | 2-methylpyrazine M | C5H6N2 | 94.1 | 1279 | 827.85 | 1.073 |
| 49 | 2-methylpyrazine D | C5H6N2 | 94.1 | 1279 | 827.75 | 1.0882 |
| 50 | 2-octanone | C8H16O | 128.2 | 1297 | 880.987 | 1.3343 |
| 51 | octanal M | C8H16O | 128.2 | 1301 | 891.341 | 1.3998 |
| 52 | octanal D | C8H16O | 128.2 | 1300 | 889.701 | 1.8242 |
| 53 | 1-hydroxy-2-propanone | C3H6O2 | 74.1 | 1306 | 906.463 | 1.0421 |
| 54 | (E)-3-hexenol | C6H12O | 100.2 | 1311 | 923.089 | 1.2369 |
| 55 | 3-methylpentanol | C6H14O | 102.2 | 1318 | 947.643 | 1.3111 |
| 56 | 2,5-dimethylpyrazine | C6H8N2 | 108.1 | 1327 | 975.184 | 1.1139 |
| 57 | (E)-2-heptenal | C7H12O | 112.2 | 1332 | 992.725 | 1.2568 |
| 58 | methyl heptenone | C8H14O | 126.2 | 1347 | 1046.964 | 1.1772 |
| 59 | dimethyl trisulfide | C2H6S3 | 126.3 | 1357 | 1081.685 | 1.3042 |
| 60 | 1-hexanol M | C6H14O | 102.2 | 1367 | 1122.538 | 1.3221 |
| 61 | 1-hexanol D | C6H14O | 102.2 | 1366 | 1117.489 | 1.6379 |
| 62 | ethyl lactate | C5H10O3 | 118.1 | 1381 | 1179.318 | 1.1433 |
| 63 | (Z)-3-hexenol M | C6H12O | 100.2 | 1393 | 1233.068 | 1.2291 |
| 64 | (Z)-3-hexenol D | C6H12O | 100.2 | 1394 | 1234.446 | 1.5094 |
| 65 | nonanal | C9H18O | 142.2 | 1398 | 1251.23 | 1.4721 |
| 66 | 2-cyclohexenone | C6H8O | 96.1 | 1404 | 1279.452 | 1.1149 |
| 67 | 2-butoxyethanol | C6H14O2 | 118.2 | 1407 | 1295.776 | 1.2919 |
| 68 | (E)-2-octenal | C8H14O | 126.2 | 1427 | 1392.429 | 1.3346 |
| 69 | trimethylpyrazine | C7H10N2 | 122.2 | 1433 | 1421.013 | 1.1679 |
| 70 | acetic acid | C2H4O2 | 60.1 | 1454 | 1532.292 | 1.0509 |
| 71 | 1-octen-3-ol | C8H16O | 128.2 | 1464 | 1585.289 | 1.1626 |
| 72 | diallyl disulfide M | C6H10S2 | 146.3 | 1465 | 1592.656 | 1.1991 |
| 73 | diallyl disulfide D | C6H10S2 | 146.3 | 1466 | 1596.792 | 1.632 |
| 74 | ethyl octanoate | C10H20O2 | 172.3 | 1467 | 1601.005 | 1.4761 |
| 75 | furfural M | C5H4O2 | 96.1 | 1468 | 1609.8 | 1.0837 |
| 76 | furfural D | C5H4O2 | 96.1 | 1468 | 1607.942 | 1.3346 |
| 77 | (E,E)-2,4-heptadienal M | C7H10O | 110.2 | 1487 | 1721.241 | 1.1879 |
| 78 | (E,E)-2,4-heptadienal D | C7H10O | 110.2 | 1487 | 1720.072 | 1.6209 |
| 79 | 2-acetylfuran | C6H6O2 | 110.1 | 1502 | 1815.286 | 1.1147 |
| 80 | (E)-2-nonenal | C9H16O | 140.2 | 1502 | 1818.222 | 1.4072 |
| 81 | benzaldehyde M | C7H6O | 106.1 | 1508 | 1858.176 | 1.1509 |
| 82 | benzaldehyde D | C7H6O | 106.1 | 1509 | 1859.845 | 1.4716 |
| 83 | bornyl acetate | C12H20O2 | 196.3 | 1565 | 2276.104 | 1.2187 |
| 84 | 5-methylfurfural | C6H6O2 | 110.1 | 1568 | 2302.57 | 1.1253 |
| 85 | methyl benzoate | C8H8O2 | 136.1 | 1575 | 2357.601 | 1.2025 |

1. The voltile compounds detected in all 18 kinds of teas by GC-IMS. The signal M represented monome, the signal D represented dimer, and the T represented Trimer.

2. RI, retention index.

3. RT, retention time.

4. DT, relative migration time.

**Table S3.** The aroma compounds in 18 kinds of teas detected by GC×GC-MS

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| no. | RI | aorma compounds | identification methods | perception | peak areas of tea samples | | | | | | | | | | | | | | | | | |
| NO.1 | NO.2 | NO.3 | NO.4 | NO.5 | NO.6 | NO.7 | NO.8 | NO.9 | NO.10 | NO.11 | NO.12 | NO.13 | NO.14 | NO.15 | NO.16 | NO.17 | NO.18 |
| 1 | 813 | 2-methylpropanal | MS/RI/S | herbal green | 1591.94 | 0.00 | 3.22 | 275.36 | 105.92 | 495.28 | 2064.99 | 186.94 | 838.85 | 0.00 | 850.65 | 129.05 | 1005.22 | 1204.56 | 1750.82 | 2866.93 | 745.62 | 1765.12 |
| 2 | 814 | acetone | MS/RI | solvent 、fruit | 252.21 | 103.02 | 293.89 | 17.18 | 81.79 | 47.77 | 777.72 | 79.11 | 325.30 | 340.62 | 113.16 | 31.49 | 0.00 | 228.36 | 41.68 | 63.24 | 0.00 | 273.10 |
| 3 | 832 | 3-methylfuran | MS/RI | chocolate | 0.00 | 0.00 | 959.66 | 107.38 | 73.10 | 13.65 | 0.00 | 133.60 | 369.92 | 0.00 | 228.48 | 155.61 | 180.22 | 0.00 | 0.00 | 959.06 | 0.00 | 566.59 |
| 4 | 864 | methyl acetate | MS/RI | green, etherial, fruity, fresh, rum and whiskey-like | 944.46 | 0.00 | 154.64 | 0.00 | 0.00 | 1.10 | 708.94 | 0.00 | 252.73 | 1805.29 | 337.70 | 0.00 | 454.80 | 2152.75 | 0.00 | 443.47 | 194.35 | 305.98 |
| 5 | 876 | 2-methylfuran | MS/RI | chocolate | 630.31 | 0.00 | 945.36 | 505.65 | 449.45 | 540.32 | 1306.35 | 436.98 | 247.98 | 1560.52 | 1730.51 | 401.71 | 1520.15 | 2822.33 | 55.64 | 60.22 | 104.10 | 1375.48 |
| 6 | 907 | ethyl acetate | MS/RI/S/O | sweet waxy floral | 2124.63 | 0.00 | 749.95 | 533.34 | 462.50 | 873.25 | 804.07 | 326.91 | 638.93 | 9543.84 | 173.31 | 316.66 | 241.90 | 0.00 | 764.25 | 0.00 | 264.71 | 208.23 |
| 7 | 910 | 3-methylbutanal | MS/RI/S/O | fruity nutty cocoa | 0.00 | 138.27 | 0.00 | 1082.47 | 2357.28 | 10.22 | 871.49 | 90.34 | 3174.00 | 0.00 | 2161.91 | 658.87 | 6088.07 | 72.69 | 7931.99 | 8120.79 | 5214.58 | 0.00 |
| 8 | 912 | 2-methylbutanal | MS/RI/S/O | cocoa, almond | 9147.84 | 0.00 | 1138.19 | 1335.77 | 0.00 | 3628.03 | 14034.04 | 6232.86 | 3715.54 | 4033.55 | 2224.08 | 0.00 | 0.00 | 8507.91 | 7125.03 | 10995.98 | 3708.87 | 13765.76 |
| 9 | 935 | pentanal | MS/RI/S/O | nutty、 cocoa | 4188.38 | 792.40 | 3156.80 | 3137.76 | 6437.30 | 4805.61 | 8300.61 | 9177.41 | 9755.67 | 2667.50 | 5947.33 | 5098.19 | 9433.92 | 4258.44 | 1237.99 | 4601.33 | 3990.48 | 5506.36 |
| 10 | 955 | 2-ethylfuran | MS/RI | solvent ethereal brown cocoa beany rooty earthy musty | 808.85 | 0.00 | 1568.94 | 1443.63 | 316.89 | 1188.28 | 1664.53 | 286.09 | 868.00 | 3433.33 | 1496.22 | 532.34 | 2076.64 | 5361.72 | 767.39 | 3451.10 | 2112.62 | 5859.01 |
| 11 | 973 | 1-penten-3-one | MS/RI/S/O | fish, pungent | 520.29 | 62.40 | 8077.05 | 376.74 | 249.83 | 295.19 | 989.61 | 436.00 | 324.06 | 2049.04 | 4287.90 | 3843.34 | 5690.77 | 3061.87 | 528.85 | 965.31 | 2110.08 | 1229.99 |
| 12 | 998 | 2,3-butanedione | MS/RI/S/O | creamy buttery | 0.00 | 0.00 | 0.00 | 83.38 | 86.05 | 14.09 | 303.72 | 76.67 | 0.00 | 80.57 | 7.67 | 0.00 | 298.04 | 209.74 | 113.61 | 0.00 | 3.42 | 0.00 |
| 13 | 1000 | amylene hydrate | MS/RI | pungent | 0.00 | 66.74 | 0.00 | 0.00 | 0.00 | 43.29 | 0.00 | 0.00 | 25.00 | 103.29 | 0.00 | 0.00 | 0.00 | 409.50 | 27.80 | 235.52 | 148.81 | 202.52 |
| 14 | 1008 | 2-methyl-3-buten-2-ol | MS/RI/S | herbal earthy oily | 0.00 | 0.00 | 36.75 | 29.04 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 15.63 | 0.00 | 0.00 | 0.00 | 9.87 | 15.92 | 34.89 |
| 15 | 1042 | toluene | MS/RI/S | sweet | 4579.93 | 1618.49 | 8015.37 | 2061.97 | 2264.03 | 1100.55 | 5816.12 | 3515.61 | 5214.73 | 13558.76 | 2674.57 | 4171.87 | 4245.35 | 17541.28 | 8032.06 | 4869.77 | 4775.10 | 2389.39 |
| 16 | 1047 | (E)-2-butenal | MS/RI/S | flower | 0.00 | 50.04 | 0.00 | 394.82 | 0.00 | 172.09 | 0.00 | 0.00 | 23.42 | 0.00 | 0.00 | 410.20 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 17 | 1054 | 2,3-pentanedione | MS/RI/S/O | cream, butter | 309.00 | 0.00 | 412.04 | 69.01 | 42.74 | 141.73 | 778.06 | 100.03 | 356.93 | 210.74 | 274.54 | 156.38 | 977.97 | 455.95 | 61.80 | 138.08 | 177.03 | 94.60 |
| 18 | 1071 | dimethyl disulfide | MS/RI/S/O | onion, cabbage | 36.83 | 0.00 | 0.00 | 39.53 | 41.06 | 37.07 | 66.05 | 45.73 | 71.58 | 0.00 | 5.18 | 0.00 | 0.00 | 0.00 | 43.07 | 251.38 | 25.63 | 89.81 |
| 19 | 1084 | hexanal | MS/RI/S/O | grass, fat | 7207.50 | 1323.65 | 13862.30 | 9140.65 | 8010.29 | 15869.62 | 14519.28 | 5754.07 | 12764.01 | 20403.47 | 26911.82 | 15671.39 | 20868.99 | 24621.05 | 10443.62 | 18252.52 | 34163.38 | 36880.96 |
| 20 | 1090 | pentanoic acid | MS/RI/S | sweat | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 6.60 | 0.00 | 0.00 | 103.21 | 149.80 | 0.00 | 148.30 | 199.32 | 282.42 | 73.97 | 244.83 | 266.85 | 431.76 |
| 21 | 1093 | 2-methylthiophene | MS/RI/S/O | sulfurous roasted green cabbage onion bitter | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 270.79 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 22 | 1101 | 2-methyl-2-butenal | MS/RI/S/O | green, fruit | 139.55 | 0.00 | 601.12 | 77.82 | 56.40 | 64.66 | 195.13 | 41.46 | 138.28 | 1261.94 | 669.63 | 85.62 | 288.45 | 1295.11 | 670.47 | 1107.81 | 258.97 | 972.85 |
| 23 | 1131 | (E)-2-pentenal | MS/RI/S/O | fruit | 70.19 | 251.07 | 15797.86 | 1127.24 | 0.00 | 854.64 | 1386.47 | 601.92 | 27.22 | 4505.37 | 4945.83 | 4725.50 | 7304.76 | 5356.29 | 917.93 | 2170.11 | 3302.51 | 5639.49 |
| 24 | 1131 | 3-heptanone | MS/RI/S/O | green, fatty, fruity | 2730.21 | 0.00 | 874.63 | 313.06 | 600.28 | 1598.27 | 1790.13 | 735.01 | 2426.63 | 208.62 | 112.55 | 271.86 | 306.90 | 413.74 | 2158.48 | 824.69 | 1953.89 | 216.31 |
| 25 | 1132 | propanoic acid, butyl ester | MS/RI/S/O | fruity, sweet | 0.00 | 0.00 | 0.00 | 55.46 | 109.19 | 0.00 | 104.69 | 87.81 | 117.10 | 0.00 | 0.00 | 0.00 | 0.00 | 59.40 | 281.44 | 0.00 | 231.73 | 0.00 |
| 26 | 1157 | 2-methyl-2-pentenal | MS/RI/S/O | sweet, fruity | 0.00 | 0.00 | 550.45 | 342.42 | 160.13 | 243.75 | 601.34 | 49.02 | 755.98 | 892.27 | 860.07 | 119.54 | 485.09 | 1066.91 | 0.00 | 1681.84 | 390.13 | 2981.97 |
| 27 | 1157 | 1-penten-3-ol | MS/RI/S/O | butter, pungent | 395.08 | 29.12 | 4422.71 | 810.65 | 96.06 | 905.33 | 2127.17 | 484.87 | 986.88 | 2241.93 | 2444.08 | 2716.20 | 4063.18 | 3717.53 | 284.02 | 1387.67 | 1654.32 | 1771.76 |
| 28 | 1158 | trans-2-butenoic acid ethyl ester | MS/RI/S/O | musty, onion, garlic, caramellic | 25.47 | 0.00 | 305.18 | 0.00 | 22.45 | 130.71 | 149.40 | 18.30 | 147.47 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 160.31 | 0.00 | 130.25 | 0.00 |
| 29 | 1166 | α-phellandrene | MS/RI/S/O | turpentine, mint, spice | 1317.18 | 0.00 | 148.23 | 0.00 | 0.00 | 211.78 | 327.32 | 42.60 | 221.13 | 812.77 | 78.20 | 226.81 | 442.29 | 570.77 | 3.20 | 1592.27 | 0.00 | 0.00 |
| 30 | 1170 | β-myrcene | MS/RI/S/O | woody, citrus | 6263.06 | 3389.08 | 1416.09 | 714.37 | 507.45 | 12327.35 | 3592.54 | 512.48 | 15696.59 | 6160.49 | 612.72 | 3147.44 | 4579.73 | 3788.24 | 17909.59 | 21053.70 | 12866.09 | 35690.32 |
| 31 | 1174 | heptanal | MS/RI/S/O | fat, citrus | 2424.10 | 718.55 | 8029.16 | 2588.24 | 2506.46 | 4741.69 | 5322.83 | 1464.02 | 3936.98 | 0.00 | 139.22 | 2984.24 | 9626.58 | 452.46 | 3063.08 | 3374.04 | 12857.53 | 8657.79 |
| 32 | 1177 | methyl hexanoate | MS/RI/S/O | tropical fruit， creamy | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 239.63 | 0.00 | 175.35 | 2078.68 | 0.00 | 0.00 | 0.00 | 4453.11 | 178.69 | 1790.64 | 0.00 | 3207.41 |
| 33 | 1178 | α-terpinene | MS/RI/S | lemon | 1790.97 | 0.00 | 122.52 | 29.67 | 41.71 | 915.16 | 366.50 | 63.68 | 622.45 | 1720.34 | 94.48 | 709.65 | 411.34 | 1141.27 | 0.00 | 1366.94 | 595.25 | 1608.07 |
| 34 | 1178 | 1-ethyl-1H-pyrrole | MS/RI/S/O | burnt | 16305.14 | 0.00 | 199.40 | 1384.14 | 603.16 | 382.97 | 5895.79 | 617.64 | 3255.09 | 6044.92 | 881.85 | 99.05 | 482.44 | 7189.33 | 754.98 | 516.67 | 107.57 | 353.92 |
| 35 | 1201 | (+)-limonene | MS/RI/S/O | citrus | 9108.46 | 5843.43 | 3323.41 | 1334.69 | 3008.01 | 51365.27 | 9801.81 | 3332.28 | 10219.72 | 16160.53 | 0.00 | 86821.33 | 9386.96 | 15783.55 | 20459.12 | 12707.34 | 11880.76 | 9962.56 |
| 36 | 1201 | (E)-2-hexenal | MS/RI/S/O | apple, green | 589.58 | 218.42 | 16127.13 | 985.31 | 199.71 | 2800.75 | 610.93 | 258.71 | 0.00 | 6633.77 | 3016.42 | 1303.65 | 2001.18 | 7797.39 | 12577.65 | 11491.75 | 20054.69 | 30916.54 |
| 37 | 1206 | 3-methyl-2-butenal | MS/RI/S/O | sweet, fruity, green | 140.36 | 0.00 | 647.38 | 192.41 | 0.00 | 88.48 | 91.47 | 290.25 | 62.82 | 381.54 | 324.26 | 254.42 | 140.45 | 300.28 | 104.38 | 215.04 | 2126.92 | 388.49 |
| 38 | 1209 | β-phellandrene | MS/RI/S/O | mint, terpentine | 1713.96 | 119.32 | 0.00 | 33.94 | 18.03 | 0.00 | 458.02 | 35.90 | 270.16 | 893.38 | 121.50 | 0.00 | 0.00 | 0.00 | 0.00 | 1722.10 | 1012.66 | 0.00 |
| 39 | 1209 | pyrazine | MS/RI/S | roasted hazelnut | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 436.83 | 135.67 | 0.00 | 0.00 | 149.06 |
| 40 | 1213 | 1,8-cineole | MS/RI/S | mint | 0.00 | 0.00 | 557.25 | 76.08 | 28.78 | 202.62 | 197.20 | 70.10 | 334.47 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 173.89 | 117.16 | 0.00 | 0.00 |
| 41 | 1220 | ethyl hexanoate | MS/RI/S | apple peel, fruit | 0.00 | 0.00 | 348.42 | 102.89 | 174.64 | 467.47 | 846.72 | 166.04 | 971.17 | 93.09 | 27.42 | 89.01 | 157.16 | 111.24 | 802.16 | 763.39 | 933.29 | 383.97 |
| 42 | 1225 | butanoic acid, butyl ester | MS/RI/S | sweet, fruity, fatty | 135.88 | 0.00 | 0.00 | 78.63 | 169.56 | 147.41 | 456.99 | 189.98 | 433.30 | 0.00 | 90.88 | 0.00 | 0.00 | 0.00 | 1002.09 | 252.50 | 762.61 | 0.00 |
| 43 | 1230 | 4-heptenal | MS/RI/S/O | biscuit, cream | 931.31 | 69.21 | 12033.39 | 597.18 | 164.72 | 535.82 | 1247.82 | 364.16 | 304.38 | 3576.66 | 1983.50 | 2927.11 | 5233.97 | 6062.87 | 505.55 | 1172.37 | 3761.46 | 1964.21 |
| 44 | 1236 | 6-methyl-2-heptanone | MS/RI/S/O | camphoreous | 0.00 | 28.85 | 182.21 | 401.54 | 0.00 | 343.99 | 260.96 | 18.38 | 184.53 | 1321.45 | 139.97 | 78.36 | 322.96 | 1540.09 | 279.30 | 460.47 | 548.67 | 796.22 |
| 45 | 1238 | γ-terpinene | MS/RI | citrus, lime-iike | 1197.24 | 121.16 | 194.07 | 121.65 | 152.63 | 5332.30 | 531.08 | 137.20 | 754.97 | 946.15 | 136.27 | 8367.72 | 910.68 | 935.72 | 1668.70 | 1212.81 | 759.36 | 1148.37 |
| 46 | 1240 | 2-pentylfuran | MS/RI/S/O | fruity, metallic | 560.38 | 160.73 | 892.23 | 476.89 | 243.99 | 1541.62 | 1585.35 | 215.16 | 746.26 | 7571.23 | 833.45 | 875.77 | 5403.40 | 9412.96 | 1975.29 | 8081.50 | 6373.03 | 10424.37 |
| 47 | 1242 | trans-β-ocimene | MS/RI | sweet, herb | 2214.73 | 723.51 | 243.29 | 89.96 | 0.00 | 3392.52 | 787.33 | 0.00 | 4621.16 | 2192.26 | 0.00 | 430.87 | 1650.19 | 1568.14 | 0.00 | 7875.44 | 4157.04 | 0.00 |
| 48 | 1243 | (E)-2-heptenal | MS/RI/S/O | soap, fatty | 0.00 | 224.01 | 8168.60 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 91.15 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 6525.66 |
| 49 | 1248 | prenyl acetate | MS/RI | sweet, banana, fruity, ripe floral, green | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 132.27 | 0.00 |
| 50 | 1251 | ocimene | MS/RI/S/O | citrus，woody | 2825.76 | 975.98 | 642.86 | 0.00 | 409.07 | 4974.65 | 1073.11 | 147.91 | 6088.38 | 2804.41 | 564.11 | 3762.31 | 9307.20 | 1783.03 | 15335.67 | 10751.45 | 5728.68 | 37077.94 |
| 51 | 1253 | methyl (Z)-3-hexenoate | MS/RI/S/O | fruity floral | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 4971.66 | 0.00 | 0.00 | 0.00 | 4572.68 | 0.00 | 0.00 | 0.00 | 0.00 |
| 52 | 1255 | 1-pentanol | MS/RI/S/O | fusel, sweet | 996.16 | 621.42 | 478.82 | 1904.27 | 1680.36 | 2798.50 | 6048.78 | 2878.58 | 4875.22 | 2109.92 | 3653.81 | 2394.60 | 4540.89 | 3530.85 | 600.93 | 3188.98 | 2854.81 | 2823.23 |
| 53 | 1258 | cis-β-hexenyl formate | MS/RI/S/O | green, waxy, fresh vegetable, fruity, apple, guava, green banana | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 97.42 | 0.00 | 0.00 | 0.00 | 137.68 | 0.00 | 0.00 | 0.00 | 0.00 | 20.99 | 0.00 | 0.00 | 221.57 |
| 54 | 1264 | methylpyrazine | MS/RI/S/O | nutty, roasted | 591.30 | 235.98 | 0.00 | 34.37 | 0.00 | 11.00 | 550.80 | 11.46 | 300.96 | 3319.94 | 68.44 | 55.21 | 46.43 | 6599.04 | 501.45 | 1543.77 | 571.55 | 83.37 |
| 55 | 1280 | hexyl acetate | MS/RI/S/O | fruity, green, fresh, sweet, banana peel, apple and pear | 0.00 | 211.80 | 194.89 | 0.00 | 0.00 | 279.23 | 173.34 | 11.39 | 309.98 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 418.56 | 0.00 | 303.54 | 1268.32 |
| 56 | 1280 | octanal | MS/RI/S/O | fat, soap, | 1141.77 | 1909.86 | 2409.84 | 2390.47 | 1275.25 | 2217.45 | 2310.93 | 840.86 | 2054.31 | 4312.61 | 1171.79 | 1320.48 | 2250.68 | 2769.45 | 1574.72 | 2324.54 | 4348.15 | 6090.24 |
| 57 | 1284 | methyl (2E)-2-hexenoate | MS/RI/S/O | fruity, green, banana, honey | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 2736.97 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1442.92 | 0.00 | 0.00 |
| 58 | 1285 | 2-octanone | MS/RI/S | dairy,cheese, | 206.35 | 0.00 | 15.27 | 18.96 | 0.00 | 194.98 | 0.00 | 48.03 | 0.00 | 1705.69 | 350.50 | 63.35 | 115.45 | 3157.34 | 311.02 | 1296.11 | 924.71 | 1589.27 |
| 59 | 1310 | (Z)-2-penten-1-ol | MS/RI/S/O | green, spicy | 246.01 | 281.30 | 6638.57 | 1023.95 | 0.00 | 1081.53 | 1868.35 | 297.82 | 1009.54 | 2617.39 | 2226.47 | 3231.79 | 3933.67 | 4569.43 | 888.32 | 2114.90 | 1785.97 | 2687.01 |
| 60 | 1313 | 1-octen-3-one | MS/RI/S/O | mushroom, metal | 0.00 | 59.32 | 705.97 | 109.72 | 326.03 | 0.00 | 964.95 | 273.84 | 584.14 | 451.86 | 234.36 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 61 | 1315 | cis-3-hexenyl-1-acetate | MS/RI/S | green fruity apple and pear, with fresh tropical nuances | 83.66 | 0.00 | 3233.19 | 21.82 | 72.47 | 3699.97 | 0.00 | 26.34 | 66.36 | 618.07 | 0.00 | 159.98 | 72.96 | 0.00 | 0.00 | 0.00 | 0.00 | 2072.38 |
| 62 | 1321 | trans-2-pentenol | MS/RI/S | mushroom | 0.00 | 0.00 | 661.31 | 48.96 | 46.59 | 66.32 | 222.74 | 19.84 | 143.65 | 341.82 | 318.21 | 278.64 | 350.03 | 30.56 | 106.58 | 208.93 | 226.42 | 294.35 |
| 63 | 1323 | 2,5-dimethylpyrazine | MS/RI/S/O | cocoa，roasted nuts，roast beef，woody grass | 0.00 | 138.02 | 0.00 | 0.00 | 0.00 | 0.00 | 3092.80 | 0.00 | 126.32 | 3667.41 | 0.00 | 0.00 | 0.00 | 8693.05 | 0.00 | 0.00 | 0.00 | 0.00 |
| 64 | 1328 | 2,6-dimethylpyrazine | MS/RI/S | meaty, nutty, roasted cocoa, brothy bready, coffee, musty | 279.25 | 0.00 | 0.00 | 28.59 | 0.00 | 0.00 | 346.18 | 0.00 | 158.77 | 0.00 | 0.00 | 0.00 | 0.00 | 2915.24 | 98.78 | 176.54 | 206.94 | 0.00 |
| 65 | 1333 | 2-ethylpyrazine | MS/RI/S/O | nutty, musty, casky, woody, potato, earthy and cocoa with a fishy nuance | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 364.26 | 0.00 | 160.99 | 3537.22 | 0.00 | 0.00 | 0.00 | 4125.35 | 0.00 | 719.97 | 100.41 | 0.00 |
| 66 | 1335 | 2,2,6-trimethyl-cyclohexanone | MS/RI/S | honey cistus | 796.38 | 184.74 | 905.10 | 536.28 | 160.93 | 841.79 | 1436.47 | 280.25 | 631.18 | 5894.43 | 1052.04 | 534.37 | 2676.50 | 10608.02 | 3927.27 | 3251.72 | 4254.31 | 4662.06 |
| 67 | 1336 | 6-methyl-5-hepten-2-one | MS/RI/S/O | green, vegetative | 2496.76 | 444.15 | 11910.47 | 4570.40 | 971.97 | 3852.20 | 4931.18 | 757.05 | 2973.85 | 24699.44 | 8831.84 | 11216.09 | 9581.00 | 22187.32 | 5244.11 | 12798.81 | 9518.79 | 17369.67 |
| 68 | 1346 | 2, 3-dimethylpyrazine | MS/RI/S | nutty，cocoa，roasted coffee，bready | 108.49 | 15.55 | 0.00 | 23.63 | 0.00 | 0.00 | 135.62 | 0.00 | 92.72 | 277.37 | 10.60 | 23.60 | 0.00 | 1281.22 | 87.00 | 268.36 | 161.24 | 0.00 |
| 69 | 1354.974287 | (Z)-3-hexenyl-2-methylbutanoate | MS/RI/S/O | herb, sweet | 141.55 | 0.00 | 403.88 | 25.27 | 74.05 | 3344.17 | 3956.62 | 21.43 | 3226.94 | 4037.11 | 220.29 | 1076.26 | 1003.89 | 1917.87 | 719.06 | 812.39 | 2036.61 | 15203.15 |
| 70 | 1360 | 1-hexanol | MS/RI/S/O | resin, flower | 0.00 | 272.63 | 1683.30 | 408.02 | 0.00 | 4129.55 | 1748.73 | 153.10 | 2645.02 | 674.66 | 612.33 | 0.00 | 1385.62 | 0.00 | 7126.98 | 4396.98 | 2889.06 | 7149.59 |
| 71 | 1377 | dimethyl trisulfide | MS/RI/S/O | sulfur, fish, cabbage | 31.95 | 0.00 | 0.00 | 0.00 | 5.97 | 0.00 | 67.49 | 0.00 | 94.72 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 36.48 | 78.34 | 0.00 | 0.00 |
| 72 | 1385 | nonanal | MS/RI/S/O | fat, citrus | 12191.92 | 2390.95 | 10508.28 | 7889.29 | 18627.91 | 14908.53 | 10159.18 | 6053.24 | 10270.10 | 9323.33 | 2889.78 | 4550.35 | 5179.11 | 6057.19 | 8584.77 | 9103.27 | 14973.70 | 10714.92 |
| 73 | 1385 | 2-ethyl-6-methylpyrazine | MS/RI/S/O | roasted hazelnut | 648.04 | 121.83 | 0.00 | 0.00 | 0.00 | 19.00 | 1169.14 | 0.00 | 162.29 | 2376.42 | 53.79 | 0.00 | 0.00 | 3496.99 | 0.00 | 442.02 | 0.00 | 0.00 |
| 74 | 1386 | (Z)-3-hexen-1-ol | MS/RI/S/O | grass | 364.55 | 768.94 | 7347.50 | 1628.34 | 1358.22 | 13397.06 | 6741.97 | 241.30 | 154.94 | 148.85 | 0.00 | 441.31 | 0.00 | 922.12 | 87.63 | 7923.37 | 7772.94 | 0.00 |
| 75 | 1392 | 2-ethyl-5-methylpyrazine | MS/RI/S/O | coffee bean，nutty，grassy，roasted | 0.00 | 0.00 | 0.00 | 52.96 | 0.00 | 50.28 | 1810.51 | 0.00 | 802.52 | 3804.11 | 0.00 | 0.00 | 0.00 | 4901.84 | 0.00 | 1034.42 | 0.00 | 0.00 |
| 76 | 1394 | 1-octen-3-ol | MS/RI/S/O | mushroom | 1965.69 | 429.86 | 3440.28 | 1747.77 | 1072.33 | 3738.20 | 9584.61 | 934.87 | 8744.19 | 5252.61 | 1806.46 | 1193.25 | 3109.49 | 6670.95 | 2944.96 | 5165.36 | 6561.57 | 6995.70 |
| 77 | 1397 | 2,4-hexadienal | MS/RI/S/O | sweet, green, waxy, aldehydic with fresh melon nuances | 25.49 | 0.00 | 230.24 | 55.46 | 11.91 | 0.00 | 62.58 | 0.00 | 35.79 | 1052.32 | 301.71 | 179.90 | 62.13 | 838.57 | 283.65 | 454.30 | 854.29 | 2398.98 |
| 78 | 1401 | (E,E)-2,4-heptadienal | MS/RI/S/O | nut, fat | 5167.55 | 312.64 | 68818.40 | 2895.33 | 801.16 | 3398.47 | 6018.18 | 1175.34 | 1780.81 | 35557.95 | 15957.48 | 17430.98 | 22625.21 | 45926.57 | 3513.04 | 7815.02 | 12779.12 | 41283.57 |
| 79 | 1410 | (E)-2-hexenol | MS/RI/S | green | 0.00 | 30.54 | 1316.78 | 0.00 | 38.15 | 3514.37 | 760.40 | 19.72 | 1148.28 | 385.69 | 0.00 | 0.00 | 0.00 | 1680.17 | 4146.75 | 1189.04 | 26.15 | 2672.28 |
| 80 | 1414 | 3-octen-2-one | MS/RI/S/O | creamy | 0.00 | 43.40 | 667.01 | 279.16 | 72.88 | 688.75 | 0.00 | 51.75 | 0.00 | 0.00 | 1182.23 | 300.23 | 551.32 | 0.00 | 0.00 | 2571.58 | 2667.89 | 8094.17 |
| 81 | 1414 | 2-ethyl-3-methylpyrazine | MS/RI/S/O | nutty peanut, musty corn-like with raw and oily nuances | 1275.77 | 21.25 | 0.00 | 0.00 | 0.00 | 0.00 | 691.62 | 0.00 | 306.27 | 4894.36 | 0.00 | 0.00 | 0.00 | 6800.97 | 0.00 | 0.00 | 0.00 | 0.00 |
| 82 | 1420 | acetic acid, 2-ethylhexyl ester | MS/RI/S/O | herbal | 1193.86 | 0.00 | 2073.81 | 834.34 | 1154.70 | 5026.00 | 5080.67 | 996.04 | 4246.88 | 0.00 | 39.76 | 81.39 | 140.38 | 249.50 | 1151.50 | 900.45 | 743.49 | 1512.99 |
| 83 | 1420 | (Z)-linalool oxide | MS/RI/S/O | flower | 0.00 | 0.00 | 2606.83 | 0.00 | 0.00 | 11920.79 | 2315.97 | 84.56 | 3604.25 | 13997.84 | 4626.74 | 2357.14 | 0.00 | 0.00 | 19776.82 | 31333.58 | 21423.15 | 24944.27 |
| 84 | 1428 | 2-propyl pyrazine | MS/RI/S/O | green，burnt | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 282.80 | 0.00 | 0.00 | 0.00 | 0.00 | 53.40 | 112.86 | 0.00 | 0.00 |
| 85 | 1431 | hexyl 2-methylbutyrate | MS/RI/S/O | waxy, unripe fruity, apple and banana | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 193.29 | 224.03 | 0.00 | 204.75 | 3174.28 | 136.81 | 146.13 | 221.41 | 2264.82 | 160.71 | 382.63 | 421.01 | 7336.18 |
| 86 | 1436 | ethyl octanoate | MS/RI/S | fruit, fat | 207.08 | 0.00 | 249.22 | 204.36 | 140.31 | 546.91 | 946.71 | 53.53 | 637.09 | 0.00 | 0.00 | 128.79 | 0.00 | 341.88 | 805.18 | 608.69 | 1099.03 | 0.00 |
| 87 | 1437 | (E)-2-octenal | MS/RI/S/O | cucumber fatty green | 1034.69 | 109.19 | 7139.11 | 1004.31 | 301.47 | 864.69 | 1228.97 | 336.59 | 366.92 | 0.00 | 2266.71 | 2022.38 | 5099.49 | 9633.99 | 1317.76 | 3621.26 | 9563.16 | 11464.11 |
| 88 | 1449 | (E)-linalool oxide | MS/RI/S/O | flower | 3278.23 | 2261.74 | 5553.24 | 390.06 | 47.03 | 18255.55 | 3841.98 | 70.12 | 6086.74 | 8011.43 | 2076.28 | 1346.25 | 16700.78 | 16704.47 | 30678.68 | 0.00 | 31774.14 | 38401.10 |
| 89 | 1450 | acetic acid | MS/RI/S/O | sour | 0.00 | 0.00 | 0.00 | 68.35 | 0.00 | 92.49 | 113.22 | 0.00 | 184.92 | 1628.18 | 303.85 | 0.00 | 322.25 | 26.32 | 864.86 | 0.00 | 0.00 | 0.00 |
| 90 | 1455 | furfural | MS/RI/S/O | bread, almond, sweet | 2440.95 | 80.86 | 972.66 | 234.03 | 72.92 | 0.00 | 854.28 | 76.56 | 200.48 | 15248.20 | 993.28 | 161.11 | 837.15 | 11116.69 | 3518.16 | 6086.16 | 1411.90 | 4167.90 |
| 91 | 1464 | cis-3-Hexenyl butyrate | MS/RI/S/O | fresh, green, oily, waxy, apple and pear | 0.00 | 0.00 | 1679.26 | 90.07 | 0.00 | 7312.63 | 4061.55 | 66.75 | 6174.84 | 3434.94 | 111.51 | 1101.41 | 1280.08 | 2520.85 | 466.98 | 1001.89 | 2310.19 | 16565.22 |
| 92 | 1465 | diallyl disulphide | MS/RI/S | green, onion | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 71.22 | 0.00 | 134.83 | 0.00 |
| 93 | 1466 | (E)-2-hexen-1-yl butyrate | MS/RI | fruity，apricot，banana | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1824.50 | 668.10 | 0.00 | 1114.52 | 1122.56 | 95.58 | 104.22 | 231.08 | 1130.00 | 0.00 | 0.00 | 378.17 | 3616.75 |
| 94 | 1467 | heptanol | MS/RI/S/O | green | 151.80 | 394.69 | 1017.15 | 506.55 | 106.80 | 3242.02 | 1369.91 | 64.71 | 2512.73 | 1532.06 | 1236.03 | 376.96 | 0.00 | 4982.62 | 362.93 | 2499.85 | 2208.60 | 4313.06 |
| 95 | 1468 | 6-methyl-5-hepten-2-ol | MS/RI | sweet, oily, green, coriander | 77.57 | 0.00 | 0.00 | 0.00 | 0.00 | 899.56 | 63.15 | 0.00 | 64.04 | 131.64 | 0.00 | 0.00 | 377.29 | 144.85 | 0.00 | 386.74 | 0.00 | 1150.07 |
| 96 | 1484 | decanal | MS/RI/S | soap, orange | 2131.24 | 1250.01 | 2093.60 | 994.47 | 468.19 | 1573.59 | 3065.63 | 707.75 | 2160.10 | 0.00 | 421.43 | 1029.82 | 1466.89 | 0.00 | 1756.22 | 2497.44 | 3802.26 | 5161.72 |
| 97 | 1487 | 2-ethyl-1-hexanol | MS/RI/S/O | sweet fatty fruity | 1821.26 | 146.29 | 1689.95 | 1415.14 | 1431.38 | 3585.65 | 4729.88 | 1849.69 | 5899.98 | 1734.04 | 536.23 | 11755.33 | 818.92 | 2883.99 | 5368.70 | 3578.26 | 4031.51 | 1176.77 |
| 98 | 1488 | α-copaene | MS/RI | wood, spice | 0.00 | 0.00 | 0.00 | 0.00 | 13.79 | 406.43 | 160.92 | 8.88 | 0.00 | 0.00 | 21.49 | 0.00 | 0.00 | 0.00 | 0.00 | 222.45 | 0.00 | 0.00 |
| 99 | 1490 | 2-acetylfuran | MS/RI/S/O | nutty and roasted with a sweet | 226.97 | 81.44 | 220.79 | 103.87 | 23.40 | 70.04 | 848.32 | 24.41 | 365.05 | 4618.61 | 231.55 | 131.70 | 231.32 | 6608.62 | 733.43 | 465.57 | 672.35 | 370.42 |
| 100 | 1493 | 2-decanone | MS/RI | orange floral fatty peach | 167.92 | 0.00 | 0.00 | 87.06 | 0.00 | 0.00 | 0.00 | 0.00 | 56.42 | 2518.65 | 109.95 | 0.00 | 92.87 | 3169.98 | 208.89 | 778.34 | 598.03 | 1599.66 |
| 101 | 1495 | benzaldehyde | MS/RI/S/O | almond, burnt sugar | 5613.92 | 2097.18 | 15227.38 | 4526.08 | 1336.45 | 9517.17 | 10397.69 | 2364.83 | 6110.26 | 36952.14 | 8415.62 | 13355.95 | 8706.01 | 39766.98 | 28802.02 | 38499.87 | 31233.08 | 44174.81 |
| 102 | 1497 | 3,5-diethyl-2-methylpyrazine | MS/RI/S | green, nutty | 332.08 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 2248.26 | 0.00 | 0.00 | 0.00 | 4682.70 | 0.00 | 0.00 | 0.00 | 0.00 |
| 103 | 1498 | pyrrole | MS/RI | sweet, nutty | 270.68 | 0.00 | 30.09 | 13.26 | 0.00 | 0.00 | 84.85 | 31.17 | 102.53 | 108.87 | 114.80 | 0.00 | 45.37 | 195.53 | 62.32 | 40.48 | 0.00 | 0.00 |
| 104 | 1506 | 3-nonen-2-one | MS/RI/S/O | spicy fatty woody | 76.46 | 0.00 | 211.58 | 95.60 | 0.00 | 85.99 | 58.58 | 0.00 | 67.98 | 3523.74 | 0.00 | 136.80 | 142.82 | 3380.81 | 289.96 | 1233.57 | 1416.32 | 4612.08 |
| 105 | 1523 | propanoic acid | MS/RI/S | acidic | 0.00 | 30.68 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 107.62 | 0.00 | 0.00 | 0.00 | 163.02 | 69.97 | 65.97 | 71.96 | 70.67 |
| 106 | 1523 | 2,6,10,10-tetramethyl-1-oxaspiro[4.5]dec-6-ene | MS/RI | tea，herbal，wet，tobacco，leaf，metallic，woody，spicy | 816.20 | 0.00 | 0.00 | 58.48 | 37.19 | 58.36 | 252.22 | 26.95 | 26.65 | 1303.26 | 98.65 | 0.00 | 668.18 | 624.91 | 1009.75 | 311.96 | 1038.50 | 2294.56 |
| 107 | 1525 | amyl hexanoate | MS/RI | sweet green fruity，pineapple apple pear，fatty | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 37.85 | 96.32 | 0.00 | 36.45 | 605.72 | 0.00 | 0.00 | 0.00 | 511.80 | 0.00 | 265.20 | 210.23 | 1785.10 |
| 108 | 1531 | 3,5-octadien-2-one | MS/RI/S/O | fruit, fat, mushroom | 21.50 | 0.00 | 2652.21 | 0.00 | 16.90 | 2239.59 | 48.31 | 42.57 | 13.29 | 14768.01 | 0.00 | 0.00 | 0.00 | 14446.46 | 28.87 | 14565.56 | 15133.44 | 0.00 |
| 109 | 1537 | linalool | MS/RI/S/O | flower, lavender | 18976.86 | 14541.94 | 12483.37 | 793.68 | 2405.59 | 51941.71 | 18061.88 | 2537.05 | 38687.22 | 20568.46 | 11181.17 | 11722.40 | 46325.43 | 12784.53 | 107057.42 | 76265.55 | 43993.54 | 70913.02 |
| 110 | 1542 | furfuryl acetate | MS/RI | estery, green banana peel, nasturtium | 55.92 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 280.95 | 0.00 | 0.00 | 0.00 | 1368.18 | 0.00 | 0.00 | 0.00 | 0.00 |
| 111 | 1544 | (E)-2-nonenal | MS/RI/S | soapy, cucumber | 0.00 | 155.81 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 40.80 | 0.00 | 0.00 | 0.00 | 654.43 | 2505.56 | 0.00 | 0.00 | 105.12 | 0.00 |
| 112 | 1547 | (Z)-2-octen-1-ol | MS/RI/S | sweet floral | 790.54 | 0.00 | 5083.86 | 0.00 | 100.69 | 0.00 | 3.74 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 202.73 | 1356.16 | 984.49 | 0.00 |
| 113 | 1553 | 1-octanol | MS/RI/S | chemical, metal, burnt | 1177.62 | 993.72 | 3307.49 | 195.96 | 774.07 | 3883.27 | 3809.54 | 596.70 | 3140.19 | 7925.03 | 0.00 | 0.00 | 0.00 | 0.00 | 1939.95 | 3020.70 | 0.00 | 8440.30 |
| 114 | 1555 | (E,E)-2,6-nonadienal | MS/RI/S | cucumber, melon, fatty | 141.00 | 116.33 | 1733.20 | 50.50 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1213.20 | 207.16 | 341.34 | 0.00 | 0.00 | 469.24 | 0.00 | 0.00 | 0.00 |
| 115 | 1560 | formic acid, octyl ester | MS/RI | orange, citrus | 0.00 | 0.00 | 0.00 | 1195.79 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1710.44 | 1909.05 | 2055.16 | 8010.10 | 0.00 | 979.74 | 5216.30 | 603.18 |
| 116 | 1560 | 5-methylfurfural | MS/RI/S/O | almond, caramel, burnt sugar | 1014.64 | 0.00 | 223.48 | 57.96 | 19.12 | 51.47 | 409.85 | 26.03 | 110.97 | 16258.14 | 432.89 | 0.00 | 184.45 | 13526.65 | 902.15 | 2659.76 | 596.67 | 0.00 |
| 117 | 1563 | (Z)-3-octen-1-ol | MS/RI | fatty， citrus | 0.00 | 0.00 | 54.35 | 0.00 | 0.00 | 187.40 | 0.00 | 0.00 | 84.58 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 118 | 1563 | 2-methylpropionic acid | MS/RI | rancid, butter, cheese | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 77.59 | 55.94 | 0.00 | 0.00 |
| 119 | 1569 | linalyl acetate | MS/RI | sweet, fruit | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 79.36 | 0.00 | 77.07 | 0.00 | 0.00 | 0.00 | 130.68 | 0.00 | 203.50 | 359.78 | 299.96 | 0.00 |
| 120 | 1570 | isocaryophyllene | MS/RI | wood | 0.00 | 0.00 | 57.35 | 0.00 | 27.45 | 0.00 | 269.52 | 0.00 | 9.52 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 121 | 1570 | (E,E)-3,5-octadien-2-one | MS/RI/S/O | fruity green grassy | 247.46 | 123.91 | 4779.86 | 1364.28 | 131.37 | 736.56 | 3374.81 | 400.98 | 1579.28 | 6974.60 | 4463.29 | 2927.81 | 6926.49 | 6578.76 | 875.88 | 7132.75 | 6117.17 | 36433.41 |
| 122 | 1575 | (E,Z)-2,6-nonadienal | MS/RI/S | cucumber, green | 0.00 | 0.00 | 972.77 | 0.00 | 12.06 | 0.00 | 0.00 | 25.81 | 13.05 | 0.00 | 0.00 | 0.00 | 425.91 | 1961.15 | 0.00 | 1756.06 | 1707.93 | 3096.69 |
| 123 | 1582 | 6-methyl-3,5-heptadiene-2-one | MS/RI/S | green, sweet, | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 71.96 | 6081.52 | 442.14 | 295.59 | 713.47 | 3768.64 | 624.69 | 2146.69 | 2865.17 | 3078.27 |
| 124 | 1590 | trans-2-decenal | MS/RI | fatty,mushroom | 0.00 | 0.00 | 620.01 | 64.91 | 26.55 | 232.77 | 0.00 | 43.57 | 37.41 | 0.00 | 297.45 | 494.30 | 0.00 | 0.00 | 0.00 | 0.00 | 27.06 | 0.00 |
| 125 | 1590 | β-cyclocitral | MS/RI/S/O | tropical saffron herbal clean rose oxide sweet tobacco damascone fruity | 2725.96 | 835.62 | 3925.47 | 1142.64 | 406.68 | 2509.72 | 3934.22 | 781.57 | 1318.09 | 16322.64 | 3136.30 | 3554.20 | 13842.42 | 14559.69 | 9245.01 | 8699.55 | 11940.99 | 18584.36 |
| 126 | 1591 | terpinen-4-ol | MS/RI | nutmeg, must | 753.16 | 0.00 | 624.14 | 36.70 | 21.27 | 526.97 | 98.20 | 31.52 | 208.94 | 1001.59 | 274.36 | 406.49 | 40.20 | 1168.92 | 0.00 | 0.00 | 0.00 | 0.00 |
| 127 | 1593 | 2-acetyl-5-methylfuran | MS/RI | nutty, cocoa, toasted bready | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 29.19 | 26.87 | 0.00 | 0.00 | 241.26 | 24.88 | 0.00 | 0.00 | 132.02 | 54.25 | 300.81 | 143.26 | 569.07 |
| 128 | 1594 | β-caryophyllene | MS/RI | wood, spice | 0.00 | 0.00 | 0.00 | 69.32 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 129 | 1595 | dimethyl sulfoxide | MS/RI/S | fatty，cheesy，garlic，mushroom | 647.70 | 135.13 | 295.34 | 138.76 | 359.28 | 367.55 | 1144.29 | 571.91 | 688.76 | 0.00 | 416.13 | 188.79 | 625.26 | 0.00 | 148.15 | 246.65 | 0.00 | 68.11 |
| 130 | 1595 | isophorone | MS/RI | sweet, citrus | 76.39 | 186.70 | 833.92 | 0.00 | 0.00 | 277.70 | 87.79 | 5.68 | 39.88 | 1850.79 | 1442.21 | 76.31 | 89.54 | 1566.19 | 154.22 | 672.84 | 809.24 | 0.00 |
| 131 | 1596 | safranal | MS/RI | woody, medicinal, phenolic, spicy and camphoreous with a fruity, herbal nuance | 2083.66 | 85.38 | 516.51 | 525.68 | 314.56 | 230.51 | 1861.77 | 319.43 | 582.51 | 10739.91 | 1094.85 | 350.38 | 1772.06 | 11845.03 | 7328.46 | 4870.45 | 10832.79 | 6996.02 |
| 132 | 1599 | hexyl hexanoate | MS/RI/S/O | herbal fresh cut grass vegetable fruity | 0.00 | 0.00 | 52.92 | 0.00 | 16.17 | 684.73 | 817.34 | 0.00 | 350.05 | 12998.32 | 715.16 | 636.23 | 1178.24 | 7662.20 | 0.00 | 0.00 | 1115.14 | 14127.32 |
| 133 | 1600 | hexadecane | MS/RI | alkane | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 156.96 | 56.89 | 0.00 | 0.00 | 0.00 | 0.00 | 219.56 | 0.00 | 1269.16 | 0.00 | 0.00 | 37.61 | 719.94 |
| 134 | 1600 | bornyl acetate | MS/RI | camphoreous, woody, mentholic, berry, soapy | 0.00 | 0.00 | 48.58 | 72.30 | 0.00 | 27.93 | 0.00 | 0.00 | 0.00 | 200.74 | 0.00 | 51.41 | 0.00 | 0.00 | 0.00 | 114.07 | 0.00 | 0.00 |
| 135 | 1602 | octyl butyrate | MS/RI | fresh waxy, fruity,floar | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 136 | 1606 | (3Z)-3-hexenyl (2E)-2-butenoate | MS/RI | green, vegetable | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 35.22 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 136.90 | 52.78 | 0.00 | 0.00 | 0.00 |
| 137 | 1610 | (E)-2-octenol | MS/RI/S | citrus,fatty | 0.00 | 182.36 | 26.90 | 287.74 | 43.37 | 723.49 | 2197.86 | 157.09 | 2394.25 | 1111.46 | 199.17 | 377.00 | 358.89 | 1535.61 | 0.00 | 0.00 | 0.00 | 1456.04 |
| 138 | 1615 | (E,E)-2,4-octadienal | MS/RI | green，fruity，melon，citrus，fatty，tallow | 0.00 | 0.00 | 549.86 | 41.60 | 0.00 | 0.00 | 71.87 | 0.00 | 31.11 | 1040.53 | 8.53 | 146.89 | 0.00 | 1257.61 | 163.29 | 0.00 | 0.00 | 1168.21 |
| 139 | 1616 | 1-ethyl-1H-pyrrole-2-carboxaldehyde | MS/RI/S/O | burnt | 19832.33 | 177.93 | 0.00 | 0.00 | 764.47 | 126.37 | 7039.34 | 0.00 | 2688.52 | 39728.28 | 1140.96 | 82.30 | 3023.65 | 0.00 | 0.00 | 15317.71 | 4429.64 | 4176.47 |
| 140 | 1616 | β-terpineol | MS/RI | pungent earthy woody | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 70.03 | 0.00 | 0.00 | 0.00 |
| 141 | 1616 | 5H-5-methyl-6,7-dihydrocyclopentapyrazine | MS/RI | musty, nutty, roasted and grainy with coffee notes | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 20.83 | 0.00 | 0.00 | 400.49 | 0.00 | 0.00 | 0.00 | 499.47 | 0.00 | 0.00 | 0.00 | 0.00 |
| 142 | 1619 | carbitol | MS/RI | slightly ethereal | 146.45 | 0.00 | 57.88 | 11.39 | 0.00 | 29.39 | 0.00 | 17.02 | 30.36 | 144.01 | 78.10 | 139.83 | 0.00 | 0.00 | 40.23 | 0.00 | 0.00 | 128.48 |
| 143 | 1619 | butanoic acid | MS/RI/S | rancid, cheese, sweat | 0.00 | 0.00 | 0.00 | 22.17 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 144 | 1620 | p-menth-1-en-9-al | MS/RI | spicy，herbal | 203.79 | 0.00 | 0.00 | 0.00 | 0.00 | 136.71 | 116.98 | 0.00 | 16.17 | 233.18 | 200.88 | 0.00 | 0.00 | 1978.52 | 832.09 | 562.13 | 198.99 | 418.01 |
| 145 | 1622 | 2-methyl-benzaldehyde | MS/RI | cherry | 173.91 | 39.21 | 443.54 | 119.56 | 19.54 | 46.06 | 488.54 | 76.70 | 72.15 | 715.91 | 0.00 | 0.00 | 38.47 | 3639.54 | 206.31 | 0.00 | 27.61 | 0.00 |
| 146 | 1622 | 2-acetyl pyrazine | MS/RI | popcorn，chocolate，hazelnut，coffee | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 160.46 | 0.00 | 0.00 | 0.00 | 405.49 | 0.00 | 0.00 | 0.00 | 0.00 |
| 147 | 1622 | linalyl isobutyrate | MS/RI | floral, fruity, sweet, berry, citrus | 0.00 | 0.00 | 0.00 | 39.24 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 148 | 1625 | phenylethanal | MS/RI/S/O | honey, sweet | 380.10 | 714.69 | 2100.38 | 382.04 | 373.65 | 1104.85 | 2591.04 | 1013.84 | 1428.06 | 9561.37 | 11646.94 | 60941.27 | 8762.51 | 10684.54 | 26447.33 | 41634.39 | 29539.64 | 38919.09 |
| 149 | 1626 | 1-methyl-1H-pyrrole-2-carboxaldehyde | MS/RI | roasted nutty | 17.01 | 0.00 | 0.00 | 127.21 | 90.20 | 23.34 | 922.11 | 27.81 | 0.00 | 949.00 | 0.00 | 65.13 | 0.00 | 2393.23 | 142.15 | 0.00 | 0.00 | 208.70 |
| 150 | 1627 | 3-methyl-benzaldehyde | MS/RI | fruity, nutty | 0.00 | 0.00 | 0.00 | 35.89 | 0.00 | 55.21 | 287.60 | 42.53 | 0.00 | 0.00 | 349.53 | 246.97 | 0.00 | 609.25 | 630.90 | 0.00 | 1091.45 | 243.43 |
| 151 | 1631 | menthol | MS/RI | minty | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 226.83 | 0.00 |
| 152 | 1636 | 2-hydroxybenzaldehyde | MS/RI | spicy, medicinal and astringent | 0.00 | 0.00 | 680.83 | 0.00 | 0.00 | 107.55 | 0.00 | 0.00 | 0.00 | 675.95 | 0.00 | 0.00 | 0.00 | 633.48 | 0.00 | 0.00 | 1513.05 | 0.00 |
| 153 | 1645 | acetophenone | MS/RI/S | bitter almond | 0.00 | 155.12 | 2647.52 | 522.59 | 355.54 | 1757.49 | 2479.69 | 640.72 | 2588.18 | 7149.44 | 0.00 | 0.00 | 0.00 | 8305.25 | 6532.14 | 0.00 | 44.26 | 0.00 |
| 154 | 1646 | alloaromadendrene | MS/RI | woody | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 40.17 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 36.67 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 155 | 1646 | 3-hexenyl hexanoate | MS/RI/S/O | green, fruity, fatty, tropical and pulpy with citrus | 243.73 | 69.36 | 0.00 | 99.80 | 1430.91 | 8618.12 | 13040.56 | 217.57 | 8808.01 | 21212.07 | 1391.28 | 4356.86 | 5486.03 | 7501.28 | 1004.80 | 0.00 | 6166.10 | 33066.93 |
| 156 | 1646 | α-caryophyllene | MS/RI/S | woody | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 89.96 | 52.37 | 0.00 | 32.24 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 31.36 | 32.88 |
| 157 | 1647 | γ-butyrolactone | MS/RI | caramel, fatty | 297.13 | 0.00 | 232.24 | 54.45 | 27.43 | 66.90 | 250.04 | 173.92 | 130.34 | 0.00 | 152.75 | 125.70 | 0.00 | 266.02 | 279.38 | 0.00 | 219.21 | 180.22 |
| 158 | 1648 | dehydrolinalool | MS/RI/S/O | mouldy | 12891.50 | 0.00 | 2698.66 | 126.84 | 107.79 | 3209.27 | 5237.56 | 965.88 | 2189.70 | 14954.26 | 27434.87 | 3419.78 | 11075.60 | 3983.12 | 8733.97 | 31301.23 | 10376.20 | 28837.41 |
| 159 | 1653 | para-tolualdehyde | MS/RI | fruity，cherry | 0.00 | 0.00 | 0.00 | 0.00 | 36.31 | 0.00 | 130.89 | 19.04 | 348.68 | 3188.42 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 222.00 | 1702.60 |
| 160 | 1655 | 4-allylanisole | MS/RI | licorice, anise | 93.92 | 0.00 | 200.39 | 45.61 | 61.55 | 168.91 | 192.38 | 0.00 | 146.53 | 0.00 | 0.00 | 109.28 | 42.05 | 0.00 | 249.99 | 156.74 | 391.23 | 319.61 |
| 161 | 1657 | 2,6-octadienoic acid, 3,7-dimethyl-, methyl ester, (Z)- | MS/RI | floral，herbal，citrus，fruity，green，geranium | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 70.91 | 0.00 | 0.00 | 0.00 | 77.64 | 0.00 | 0.00 | 0.00 | 0.00 |
| 162 | 1658 | β-farnesene | MS/RI/S | wood, citrus, sweet | 48.04 | 0.00 | 0.00 | 0.00 | 0.00 | 154.46 | 0.00 | 0.00 | 210.71 | 7482.46 | 3022.32 | 17098.88 | 0.00 | 1132.79 | 0.00 | 0.00 | 0.00 | 0.00 |
| 163 | 1659 | furfuryl alcohol | MS/RI/S | burnt | 286.23 | 0.00 | 0.00 | 105.72 | 15.56 | 0.00 | 184.85 | 0.00 | 84.84 | 0.00 | 0.00 | 0.00 | 0.00 | 573.10 | 626.41 | 275.99 | 167.67 | 193.67 |
| 164 | 1659 | 2-butyl-2-octenal | MS/RI/S | green vegetable, leafy cucumber, oily, herbal, fatty, watercress, violet | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 253.70 | 0.00 | 0.00 | 514.68 | 55.51 | 0.00 | 0.00 | 0.00 | 429.15 | 2200.58 | 765.94 | 312.38 |
| 165 | 1660 | cis-beta-farnesene | MS/RI | citrus，green | 0.00 | 0.00 | 148.86 | 0.00 | 44.99 | 248.94 | 64.25 | 0.00 | 310.36 | 0.00 | 0.00 | 0.00 | 1419.67 | 0.00 | 478.63 | 1184.99 | 692.23 | 7288.90 |
| 166 | 1660 | 6,10-dimethyl-2-undecanone | MS/RI | citronella，soapy | 0.00 | 0.00 | 42.59 | 0.00 | 0.00 | 0.00 | 157.86 | 0.00 | 0.00 | 1571.07 | 0.00 | 54.64 | 89.15 | 775.12 | 157.87 | 311.14 | 640.59 | 1160.83 |
| 167 | 1660 | (E)-2-hexen-1-yl hexanoate | MS/RI | apple，pear，kiwi，leafy | 103.17 | 0.00 | 0.00 | 0.00 | 44.54 | 0.00 | 1481.95 | 0.00 | 1164.70 | 8566.10 | 550.08 | 235.75 | 477.70 | 5612.40 | 387.50 | 0.00 | 1421.37 | 12284.13 |
| 168 | 1664 | (Z)-3-nonen-1-ol | MS/RI/S | green, fat | 0.00 | 130.46 | 600.53 | 0.00 | 27.84 | 932.18 | 367.11 | 0.00 | 707.81 | 0.00 | 0.00 | 0.00 | 1459.87 | 0.00 | 1005.65 | 3482.83 | 289.03 | 5318.51 |
| 169 | 1665 | 3-methylbutanoic acid | MS/RI/S | sweat, acid, rancid | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 180.41 | 0.00 | 0.00 | 0.00 | 0.00 | 1260.27 | 0.00 | 542.62 | 0.00 |
| 170 | 1666 | L-trans-pinocarveol | MS/RI | woody, balsamic, fennel | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 105.65 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 224.58 | 0.00 | 1933.87 | 212.76 |
| 171 | 1667 | (Z)-3,7-dimethylocta-2,6-dienal | MS/RI | lemon | 0.00 | 0.00 | 483.69 | 84.19 | 0.00 | 444.98 | 115.56 | 0.00 | 311.15 | 75.37 | 89.20 | 174.38 | 69.98 | 0.00 | 1386.44 | 6133.18 | 0.00 | 11609.30 |
| 172 | 1668 | nonanol | MS/RI/S | fat, green | 0.00 | 477.91 | 1144.70 | 151.76 | 0.00 | 2811.67 | 897.37 | 0.00 | 1838.16 | 2251.79 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 9422.97 |
| 173 | 1673 | benzyl formate | MS/RI | fresh cherry, with a berry strawberry fruity nuance | 0.00 | 0.00 | 395.02 | 32.16 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1116.05 | 0.00 | 0.00 | 0.00 | 867.69 | 0.00 | 0.00 | 0.00 | 0.00 |
| 174 | 1677 | ketoisophorone | MS/RI | citrus, floral, musty, tea like with green sweet fruity nuances | 0.00 | 0.00 | 139.07 | 77.14 | 0.00 | 62.37 | 128.72 | 9.73 | 61.47 | 0.00 | 238.35 | 86.91 | 0.00 | 0.00 | 0.00 | 0.00 | 865.80 | 0.00 |
| 175 | 1677 | trans-geranic acid methyl ester | MS/RI | waxy green fruity flower | 0.00 | 0.00 | 28.83 | 0.00 | 0.00 | 757.61 | 0.00 | 0.00 | 550.96 | 958.57 | 0.00 | 0.00 | 66.14 | 781.50 | 0.00 | 8399.15 | 1505.73 | 2487.64 |
| 176 | 1681 | geranyl formate | MS/RI/S | green, floral, citrus, waxy, fruity, apple and apricot-like | 0.00 | 0.00 | 0.00 | 0.00 | 76.98 | 15.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 670.62 | 548.61 | 4252.68 |
| 177 | 1683 | 5-ethenyldihydro-5-methyl-2(3H)-furanone | MS/RI | fruity, minty | 0.00 | 0.00 | 155.79 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 669.67 | 0.00 | 0.00 | 0.00 | 618.08 | 0.00 | 0.00 | 0.00 | 0.00 |
| 178 | 1686 | (E,E)-2,4-nonadienal | MS/RI/S | fat, green | 0.00 | 0.00 | 71.33 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1173.62 | 87.88 | 0.00 | 1203.08 | 55.20 |
| 179 | 1688 | α-terpineol | MS/RI | pine，terpene，lilac，citrus，woody，floral | 3302.55 | 0.00 | 1899.88 | 62.46 | 0.00 | 575.39 | 1428.77 | 173.60 | 0.00 | 0.00 | 0.00 | 0.00 | 4242.24 | 2850.85 | 11439.82 | 5239.07 | 0.00 | 4745.69 |
| 180 | 1694 | γ-caprolactone | MS/RI | sweet, creamy, tobacco | 0.00 | 0.00 | 0.00 | 6.95 | 0.00 | 48.26 | 260.55 | 0.00 | 81.02 | 110.78 | 667.95 | 959.46 | 381.00 | 1229.64 | 128.10 | 216.09 | 370.41 | 1218.36 |
| 181 | 1696 | propiophenone | MS/RI | fruity | 0.00 | 0.00 | 0.00 | 13.07 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 4927.79 | 204.14 | 163.61 | 0.00 | 5195.47 | 261.84 | 542.27 | 246.96 | 707.30 |
| 182 | 1706 | (Z)-3-hexen-1-yl (E)-2-hexenoate | MS/RI | fruity，herbal，artichoke，tea | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 57.01 | 86.41 | 0.00 | 0.00 | 538.43 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 157.82 | 805.36 |
| 183 | 1710 | (E,E)-2,4-decadienal | MS/RI | fat,fried and potato | 0.00 | 0.00 | 310.22 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 821.95 | 160.59 | 71.12 | 0.00 | 685.83 | 0.00 | 364.92 | 1019.42 | 0.00 |
| 184 | 1710 | 2,4-dimethylbenzaldehyde | MS/RI | naphthyl, cherry, almond, spice and vanilla | 0.00 | 0.00 | 0.00 | 20.02 | 0.00 | 14.98 | 0.00 | 0.00 | 37.32 | 3201.59 | 273.80 | 0.00 | 0.00 | 165.28 | 1083.58 | 0.00 | 2071.61 | 3399.89 |
| 185 | 1714 | benzyl acetate | MS/RI | sweet，floral，fruity，jasmin，fresh | 0.00 | 0.00 | 19.46 | 98.48 | 0.00 | 142.59 | 72.55 | 0.00 | 35.94 | 4045.27 | 0.00 | 88.22 | 0.00 | 2848.07 | 1112.95 | 848.46 | 1935.49 | 1460.76 |
| 186 | 1714 | β-bisabolene | MS/RI | balsamic | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 23.64 | 2141.62 | 572.98 | 3259.32 | 260.26 | 0.00 | 52.66 | 69.35 | 69.59 | 1644.32 |
| 187 | 1715 | (Z)-3-hexen-1-yl (Z)-3-hexenoate | MS/RI/S/O | green，tomato，leaf，pear，melon，metallic，fennel，tropical | 57.32 | 0.00 | 114.50 | 0.00 | 200.07 | 1614.91 | 1021.48 | 0.00 | 631.38 | 2334.09 | 103.92 | 130.27 | 210.63 | 622.47 | 0.00 | 220.30 | 376.82 | 2387.57 |
| 188 | 1715 | (E)-citral | MS/RI/S | lemon, mint | 87.09 | 0.00 | 1337.52 | 161.00 | 0.00 | 1634.31 | 324.36 | 0.00 | 1593.09 | 2755.44 | 0.00 | 0.00 | 371.81 | 1637.07 | 2829.03 | 7687.02 | 4450.33 | 18420.46 |
| 189 | 1717 | citral | MS/RI/S | lemon | 0.00 | 462.55 | 0.00 | 0.00 | 18.91 | 25.30 | 17.57 | 11.74 | 24.94 | 0.00 | 189.01 | 318.50 | 0.00 | 0.00 | 43.63 | 1628.43 | 0.00 | 0.00 |
| 190 | 1718 | carvone | MS/RI/S | minty | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 308.12 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 237.07 | 0.00 | 0.00 | 73.46 | 0.00 | 69.37 | 0.00 |
| 191 | 1718 | naphthalene | MS/RI | tar | 596.90 | 97.13 | 566.20 | 332.95 | 127.84 | 695.59 | 955.53 | 0.00 | 384.11 | 0.00 | 218.72 | 520.39 | 385.75 | 2442.52 | 1530.70 | 1346.65 | 2401.58 | 0.00 |
| 192 | 1720 | epoxylinalol | MS/RI | floral, honey | 0.00 | 0.00 | 0.00 | 5.57 | 12.73 | 8.50 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 187.01 | 0.00 | 111.68 | 0.00 |
| 193 | 1722 | dodecanal | MS/RI | soapy, fat, citrus | 0.00 | 0.00 | 100.01 | 0.00 | 29.33 | 0.00 | 0.00 | 0.00 | 0.00 | 439.78 | 0.00 | 20.87 | 0.00 | 200.27 | 118.49 | 202.74 | 456.15 | 915.91 |
| 194 | 1722 | 2-thiophenecarboxaldehyde | MS/RI/S | sulfurous | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 110.08 | 26.03 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 577.05 | 0.00 | 552.42 | 0.00 | 0.00 |
| 195 | 1730 | δ-cadinene | MS/RI | thyme herbal woody dry | 113.33 | 54.46 | 54.77 | 20.21 | 289.28 | 3052.98 | 1396.48 | 201.83 | 451.07 | 220.40 | 163.43 | 0.00 | 199.22 | 0.00 | 244.88 | 10083.47 | 569.88 | 1853.40 |
| 196 | 1731 | 3,6-(E,Z)-Nonadien-1-ol | MS/RI | fresh green, waxy, melon, with fruity pear notes | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 119.53 | 0.00 | 0.00 | 0.00 | 0.00 | 25.95 | 0.00 | 194.78 | 0.00 | 161.34 | 1452.22 | 226.64 | 999.39 |
| 197 | 1741 | (E)-linalool oxide (pyranoid) | MS/RI/S/O | woody | 487.67 | 438.78 | 369.19 | 67.27 | 202.44 | 4789.10 | 1671.02 | 200.73 | 2457.91 | 4002.92 | 2547.11 | 1095.53 | 3230.61 | 1838.38 | 10543.09 | 17411.31 | 11017.36 | 21123.30 |
| 198 | 1745 | 2(5H)-furanone | MS/RI/S | buttery | 62.23 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 130.30 | 0.00 | 0.00 | 0.00 |
| 199 | 1745 | methyl salicylate | MS/RI/S/O | peppermint | 1479.34 | 1144.03 | 4935.90 | 175.61 | 58.60 | 12756.85 | 4690.50 | 216.91 | 5352.75 | 15710.86 | 1276.76 | 3378.56 | 8452.28 | 11085.14 | 30663.37 | 28228.38 | 18741.17 | 54968.35 |
| 200 | 1748 | α-farnesene | MS/RI | citrus herbal | 0.00 | 0.00 | 55.29 | 0.00 | 0.00 | 33.51 | 0.00 | 0.00 | 67.27 | 2760.69 | 902.77 | 7090.74 | 9635.10 | 0.00 | 171.30 | 226.37 | 0.00 | 3134.49 |
| 201 | 1749 | methyl 2-phenylacetate | MS/RI | floral, honey, spice, waxy and sweet | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 16.27 | 45.18 | 11.08 | 22.27 | 2569.46 | 99.34 | 39.48 | 0.00 | 3514.35 | 140.84 | 368.29 | 201.69 | 0.00 |
| 202 | 1754 | citronellol | MS/RI | floral, citrus | 0.00 | 0.00 | 0.00 | 30.14 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 520.77 | 794.55 | 0.00 | 16.24 |
| 203 | 1755 | 2-undecenal | MS/RI | citrus , soapy | 0.00 | 0.00 | 0.00 | 0.00 | 104.80 | 0.00 | 0.00 | 0.00 | 0.00 | 424.07 | 99.06 | 0.00 | 144.67 | 0.00 | 0.00 | 272.43 | 539.04 | 1212.84 |
| 204 | 1770 | nerol | MS/RI/S/O | sweet | 1575.56 | 418.41 | 912.23 | 0.00 | 123.65 | 2246.50 | 229.12 | 105.53 | 1079.58 | 1542.86 | 729.55 | 1318.02 | 1000.20 | 5591.35 | 3293.39 | 7650.89 | 3479.02 | 123818.97 |
| 205 | 1770 | γ-heptalactone, 4-heptanolide | MS/RI | nut, fat, fruit | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 17.23 | 0.00 | 4.15 | 0.00 | 0.00 | 0.00 | 0.00 | 218.42 | 0.00 | 0.00 | 0.00 | 0.00 |
| 206 | 1771 | benzyl isobutanoate | MS/RI | fruity, sweet, ripe berry | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 192.48 |
| 207 | 1773 | α-curcumene | MS/RI | herb | 44.34 | 0.00 | 253.68 | 0.00 | 13.26 | 193.56 | 150.18 | 0.00 | 182.12 | 1846.54 | 201.38 | 1088.35 | 288.65 | 919.93 | 318.00 | 401.74 | 787.01 | 708.72 |
| 208 | 1775 | phenethyl formate | MS/RI | sweet, green, watercress, unripe banana, narcissus, phenolic | 0.00 | 0.00 | 0.00 | 36.84 | 0.00 | 31.66 | 0.00 | 13.47 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 323.36 | 0.00 | 441.19 | 0.00 |
| 209 | 1776 | 2-phenyl-2-propanol | MS/RI | sweet | 82.75 | 0.00 | 0.00 | 36.14 | 0.00 | 1.13 | 23.16 | 0.00 | 133.74 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 210 | 1778 | α-methylphenethyl alcohol | MS/RI | sweet, pineapple | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 28.60 | 0.00 | 0.00 |
| 211 | 1782 | β-sesquiphellandrene | MS/RI | wood | 269.70 | 198.31 | 0.00 | 0.00 | 0.00 | 0.00 | 56.29 | 0.00 | 304.25 | 352.32 | 61.15 | 494.03 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 206.93 |
| 212 | 1784 | (Z)-4-decen-1-ol | MS/RI | waxy, fatty, fruity | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 139.20 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 213 | 1791 | phenylethyl acetate | MS/RI | floral，rose，sweet，honey，fruity ，tropical | 144.73 | 0.00 | 0.00 | 21.70 | 8.77 | 93.13 | 0.00 | 0.00 | 43.28 | 4781.14 | 300.06 | 430.42 | 0.00 | 2693.33 | 833.26 | 1364.29 | 931.33 | 2430.18 |
| 214 | 1794 | 4-acetyltoluene | MS/RI | sweet, creamy, fruity, cherry | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 68.16 | 0.00 | 0.00 | 506.03 |
| 215 | 1797 | 2,4-decadienal | MS/RI | orange，sweet，fresh，citrus，fatty | 0.00 | 0.00 | 113.20 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 121.76 | 126.06 | 709.28 | 150.70 | 298.69 | 418.08 | 2074.75 |
| 216 | 1803 | hexyl octanoate | MS/RI | green, apple, fruity, berry，fresh | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 186.53 |
| 217 | 1804 | methyl laurate | MS/RI | fatty coconut | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 10.51 | 0.00 | 21.08 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 187.34 |
| 218 | 1807 | (E)-2-dodecenal | MS/RI | fatty, sweet | 0.00 | 0.00 | 141.50 | 0.00 | 0.00 | 0.00 | 0.00 | 11.44 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 219 | 1811 | (E)-geranyl acetone | MS/RI | floral fruity | 3736.11 | 0.00 | 0.00 | 0.00 | 306.80 | 1956.69 | 0.00 | 0.00 | 0.00 | 0.00 | 872.26 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 220 | 1814 | 2-tridecanone | MS/RI | fatty, earthy, dairy, ketonic, cheesy | 55.47 | 0.00 | 56.62 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 73.28 | 42.89 | 50.36 | 57.61 | 82.78 |
| 221 | 1814 | (E)-beta-damascenone | MS/RI/S/O | apple rose honey tobacco sweet | 311.89 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 47.17 | 13.10 | 0.00 | 1571.69 | 132.83 | 17.83 | 0.00 | 448.10 | 5627.31 | 2067.99 | 1427.41 | 1711.68 |
| 222 | 1815 | anethole | MS/RI | sweet, anise, licorice, medicinal | 0.00 | 0.00 | 371.56 | 27.16 | 33.43 | 0.00 | 326.25 | 61.57 | 228.62 | 0.00 | 0.00 | 86.22 | 0.00 | 0.00 | 0.00 | 223.27 | 0.00 | 0.00 |
| 223 | 1815 | nerylacetone | MS/RI | fatty, metallic | 0.00 | 0.00 | 9653.70 | 1123.30 | 116.88 | 355.44 | 1774.30 | 211.78 | 1440.93 | 0.00 | 0.00 | 2967.31 | 2335.77 | 0.00 | 5729.71 | 9621.92 | 0.00 | 18744.57 |
| 224 | 1817 | cis-anethole | MS/RI | sweet anise licorice medicinal | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 65.16 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 225 | 1820 | α-methylbenzyl alcohol | MS/RI | chemical, medicinal, with a balsamic vanilla woody nuance | 0.00 | 0.00 | 0.00 | 19.85 | 0.00 | 34.57 | 0.00 | 0.00 | 0.00 | 67.97 | 0.00 | 0.00 | 0.00 | 0.00 | 83.83 | 0.00 | 260.78 | 0.00 |
| 226 | 1822 | undecanol | MS/RI | soapy waxy sweet | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 171.74 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 764.64 | 0.00 |
| 227 | 1823 | dec-2-en-1-ol | MS/RI | waxy, fresh air, citrus, rose rue | 286.06 | 0.00 | 0.00 | 63.34 | 0.00 | 0.00 | 0.00 | 0.00 | 25.06 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 10.37 | 0.00 |
| 228 | 1824 | beta-damascone | MS/RI/S/O | fruity，floral，black currant，plum，rose，honey，tobacco | 0.00 | 0.00 | 269.16 | 0.00 | 0.00 | 0.00 | 18.18 | 0.00 | 0.00 | 565.43 | 21.84 | 35.46 | 58.11 | 171.80 | 19.98 | 121.41 | 207.36 | 122.31 |
| 229 | 1824 | tridecanal | MS/RI | flower, sweet | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 57.95 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 230 | 1827 | 6,6-dimethyl-2-norpinene-2-ethanol | MS/RI | sweet, balsamic, citrus, pine, herbal | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 81.37 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 231 | 1829 | hexanoic acid | MS/RI/S/O | sour fatty | 94.20 | 0.00 | 158.99 | 0.00 | 0.00 | 282.41 | 240.93 | 0.00 | 77.76 | 6272.49 | 424.44 | 576.23 | 0.00 | 5150.91 | 2003.24 | 5589.32 | 5636.27 | 0.00 |
| 232 | 1832 | phenethyl pivalate | MS/RI | balsamic, tea, rose, spicy, geranium, green grassy, waxy | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 52.45 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 233 | 1833 | 1-furfuryl pyrrole | MS/RI/S/O | vegetative, onion, sharp and metallic | 464.52 | 0.00 | 27.34 | 0.00 | 0.00 | 9.09 | 93.79 | 0.00 | 66.09 | 3118.10 | 29.16 | 17.59 | 0.00 | 2235.60 | 51.08 | 262.77 | 21.85 | 54.27 |
| 234 | 1838 | (Z)-3-hexen-1-yl octanoate | MS/RI | green，fruity，winey，oily，asparagus，artichoke，metallic | 0.00 | 0.00 | 0.00 | 0.00 | 22.62 | 74.56 | 56.57 | 0.00 | 114.84 | 0.00 | 0.00 | 65.37 | 0.00 | 80.80 | 0.00 | 0.00 | 0.00 | 556.23 |
| 235 | 1841 | 4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)butan-2-one | MS/RI | floral | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 14.64 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 236 | 1842 | ionone | MS/RI | violet sweet floral woody | 36.14 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 6773.72 | 0.00 | 0.00 | 0.00 | 0.00 |
| 237 | 1846 | carveol | MS/RI | minty, green weedy, herbal, plastic, spicy, earthy, mahogany | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 85.85 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 129.99 | 83.22 | 140.05 | 92.46 | 148.80 | 79.10 | 0.00 |
| 238 | 1850 | 2-hexanoylfuran | MS/RI | sweet, fruity, green, waxy, beany | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 15.21 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 239 | 1851 | 2-furanacrolein | MS/RI | green grassy, fruity, spicy, vanilla, nutty, woody, cinnamon | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 262.52 | 0.00 | 0.00 | 0.00 | 297.30 | 0.00 | 0.00 | 0.00 | 0.00 |
| 240 | 1853 | trans-2-Hexenyl n-octanoate | MS/RI | pear | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 20.42 | 0.00 | 0.00 | 0.00 | 0.00 |
| 241 | 1854 | dihydro-β-Ionone | MS/RI | FLORAL,woody, seedy, berry raspberry, with leafy, spicy nuances | 90.49 | 0.00 | 0.00 | 8.49 | 0.00 | 0.00 | 0.00 | 0.00 | 19.86 | 0.00 | 25.07 | 0.00 | 0.00 | 291.79 | 325.88 | 460.06 | 438.54 | 0.00 |
| 242 | 1854 | dihydro-α-ionone | MS/RI | creamy, berry, floral, woody, orris, earthy, violet | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 65.02 | 0.00 | 0.00 | 0.00 |
| 243 | 1855 | 1-methyl-naphthalene | MS/RI | chemical | 0.00 | 0.00 | 0.00 | 45.73 | 34.80 | 0.00 | 202.07 | 57.90 | 155.44 | 0.00 | 0.00 | 0.00 | 54.82 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 244 | 1857 | methyl β-phenylpropionate | MS/RI | honey, fruity, wine, balsam, floral | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 379.95 | 0.00 | 0.00 | 0.00 | 0.00 |
| 245 | 1860 | geraniol | MS/RI/S/O | floral, rosy, waxy and perfumey with a fruity, peach-like nuance | 0.00 | 11419.54 | 1682.13 | 1458.19 | 0.00 | 33944.61 | 6681.58 | 0.00 | 44227.66 | 13807.54 | 0.00 | 0.00 | 10166.37 | 0.00 | 29200.31 | 55092.42 | 35166.46 | 0.00 |
| 246 | 1861 | 2’, 4’-dimethylacetophenone | MS/RI | floral，woody，sweet，mimosa，minty | 0.00 | 0.00 | 41.75 | 0.00 | 46.45 | 25.61 | 9.07 | 79.30 | 0.00 | 1170.70 | 31.49 | 0.00 | 0.00 | 58.47 | 35.13 | 0.00 | 0.00 | 0.00 |
| 247 | 1862 | o-guaiacol | MS/RI | phenolic, smoke, spice, vanilla, woody | 0.00 | 0.00 | 0.00 | 38.90 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 27.03 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 23.74 | 40.08 | 0.00 |
| 248 | 1863 | α-Ionone | MS/RI/S/O | sweet, woody, floral, violet, orris, tropical fruity | 0.00 | 448.06 | 10464.85 | 0.00 | 0.00 | 6.63 | 1280.73 | 0.00 | 1117.79 | 0.00 | 863.36 | 0.00 | 0.00 | 12411.77 | 0.00 | 284.97 | 0.00 | 0.00 |
| 249 | 1865 | benzyl alcohol | MS/RI/S/O | sweet, flower | 295.32 | 1763.20 | 1752.96 | 1318.86 | 178.61 | 6415.53 | 1801.29 | 92.62 | 1387.87 | 5020.91 | 980.33 | 1411.99 | 2080.08 | 3999.10 | 8811.32 | 11995.50 | 16682.58 | 20256.25 |
| 250 | 1867 | p-acetylethylbenzene | MS/RI | floral, hawthorn | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 12.03 | 0.00 | 0.00 | 50.10 | 0.00 | 0.00 | 99.58 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 251 | 1877 | 2-methyl-naphthalene | MS/RI | sweet floral | 0.00 | 0.00 | 0.00 | 0.00 | 71.36 | 0.00 | 0.00 | 58.94 | 47.11 | 0.00 | 122.54 | 0.00 | 122.98 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 252 | 1877 | Propanoic acid, 2-methyl-, 2-phenylethyl ester | MS/RI | honey, floral, fruity, tea, rose,peach,pastry | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1560.69 | 676.79 | 615.84 | 56.71 | 593.87 | 0.00 | 0.00 | 0.00 | 0.00 |
| 253 | 1879 | Furfural acetone | MS/RI | sweet, nutty, powdery, vanilla, coumarin, creamy | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 53.58 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 254 | 1881 | γ-octalactone | MS/RI | coconut，fatty | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 38.77 | 0.00 | 0.00 | 1021.12 | 114.07 | 140.38 | 0.00 | 415.47 | 0.00 | 118.96 | 180.67 | 590.01 |
| 255 | 1885 | dihydropseudoionone | MS/RI | floral, fruity, tropical, green pear apple banana citrus | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 19742.78 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 91.77 |
| 256 | 1894 | butanoic acid, 3-methyl-, phenylmethyl ester | MS/RI | sweet，fruity，apple，pineapple，herbal | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 518.66 | 0.00 | 38.98 | 0.00 | 0.00 | 0.00 | 0.00 | 277.10 | 0.00 |
| 257 | 1895 | dimethyl sulfone | MS/RI | sulfur, burnt | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 76.74 | 10.44 | 0.00 | 0.00 | 0.00 |
| 258 | 1895 | geranyl isovalerate | MS/RI | fruit, rose, apple | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 274.64 | 0.00 | 0.00 |
| 259 | 1899 | trans-2-undecen-1-ol | MS/RI | floral, rose, waxy, fresh fruity | 78.09 | 0.00 | 264.60 | 0.00 | 0.00 | 65.86 | 0.00 | 0.00 | 174.06 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 213.85 | 510.58 |
| 260 | 1907 | benzeneacetaldehyde, α-ethylidene | MS/RI | green, vegetative, floral, cocoa and nutty | 122.24 | 0.00 | 0.00 | 0.00 | 0.00 | 9.82 | 64.85 | 0.00 | 0.00 | 1715.76 | 91.83 | 105.96 | 0.00 | 1048.19 | 3328.15 | 3443.03 | 1932.26 | 3774.36 |
| 261 | 1910 | 2,6-di-tert-butyl-p-methylphenol | MS/RI | mild phenolic camphor | 198.31 | 97.79 | 202.73 | 0.00 | 0.00 | 45.21 | 54.64 | 0.00 | 54.69 | 294.78 | 64.83 | 55.04 | 98.46 | 194.06 | 207.24 | 228.36 | 236.30 | 352.96 |
| 262 | 1912 | 2-phenylethanol | MS/RI/S/O | floral, sweet, rosey and bready | 0.00 | 1387.55 | 784.84 | 1007.22 | 136.76 | 7477.69 | 1698.71 | 181.62 | 1641.94 | 11422.80 | 6694.73 | 16387.96 | 2507.01 | 3231.53 | 14786.78 | 33307.05 | 21157.21 | 30291.35 |
| 263 | 1914 | cubebol | MS/RI | spicy, minty | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 54.58 | 38.42 | 0.00 | 4.33 | 85.56 | 0.00 | 9.47 | 0.00 | 0.00 | 88.17 | 0.00 | 64.79 | 45.59 |
| 264 | 1916 | α-calacorene | MS/RI | woody | 0.00 | 0.00 | 77.27 | 0.00 | 0.00 | 35.40 | 85.38 | 0.00 | 26.79 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 221.82 | 1996.72 | 262.91 | 773.52 |
| 265 | 1917 | β-Lonone | MS/RI/S/O | woody, floral, berry, fruity | 4498.02 | 1596.90 | 7952.29 | 1145.08 | 230.55 | 2057.47 | 5342.28 | 883.39 | 1526.95 | 22400.27 | 3934.08 | 4941.61 | 4177.54 | 14914.45 | 11652.62 | 14028.20 | 20241.21 | 28705.46 |
| 266 | 1920 | benzeneacetaldehyde, α-(2-methylpropylidene)- | MS/RI | sweet，cocoa，nutty，rose，powdery | 52.48 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 686.22 | 0.00 | 0.00 | 0.00 | 368.47 | 2205.45 | 2329.52 | 1119.41 | 1107.10 |
| 267 | 1927 | calamenene | MS/RI | herb, spice | 0.00 | 32.82 | 0.00 | 0.00 | 147.51 | 1334.44 | 968.78 | 82.15 | 116.30 | 655.23 | 0.00 | 52.22 | 63.95 | 59.22 | 0.00 | 0.00 | 0.00 | 1246.34 |
| 268 | 1928 | isoamyl benzoate | MS/RI | sweet, fruity with a green tropical nuance | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 209.05 | 0.00 | 13.90 | 0.00 | 101.22 | 0.00 | 0.00 | 0.00 | 81.12 |
| 269 | 1936 | 3-Phenyl-1-propanol, acetate | MS/RI | balsamic, floral, fruity, sappy, spicy and cinnamic | 0.00 | 0.00 | 0.00 | 62.10 | 0.00 | 0.00 | 0.00 | 31.12 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 270 | 1940 | Piperitenone oxide | MS/RI | herbal, minty | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 159.28 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 72.97 | 0.00 |
| 271 | 1945 | cis-3-hexenoic acid | MS/RI | green grass, sweaty, fruity, cheesy acid | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 356.32 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 102.87 |
| 272 | 1955 | heptanoic acid | MS/RI/S | cheesy, fruity, fatty | 0.00 | 0.00 | 35.81 | 0.00 | 0.00 | 0.00 | 25.82 | 0.00 | 0.00 | 689.41 | 0.00 | 32.00 | 0.00 | 687.32 | 278.57 | 267.92 | 722.42 | 831.69 |
| 273 | 1956 | creosol | MS/RI | vaniila, spice, woody | 0.00 | 0.00 | 0.00 | 2.45 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 274 | 1956 | benzothiazole | MS/RI | meaty, beefy and coffee-like | 0.00 | 0.00 | 0.00 | 14.11 | 40.32 | 85.67 | 70.34 | 48.39 | 139.53 | 505.16 | 0.00 | 96.23 | 0.00 | 418.41 | 252.86 | 350.09 | 0.00 | 345.38 |
| 275 | 1958 | 2-phenylethyl butanoate | MS/RI | fruity, floral, green, winey | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 3563.06 | 0.00 | 1332.02 | 165.30 | 82.13 | 243.03 | 468.15 | 314.29 | 2424.03 |
| 276 | 1967 | beta-ionone epoxide | MS/RI | fruity, sweet, berry, woody, violet, orris, powdery | 331.78 | 702.61 | 1229.43 | 190.56 | 0.00 | 343.20 | 796.35 | 48.12 | 200.13 | 5661.50 | 869.31 | 1505.37 | 660.68 | 4101.97 | 797.89 | 1802.17 | 4478.29 | 5327.15 |
| 277 | 1968 | butanoic acid, 2-methyl-, 2-phenylethyl ester | MS/RI | fruity, floral, green, sweet, waxy | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 5.72 | 1929.09 | 263.10 | 2940.92 | 95.77 | 0.00 | 0.00 | 0.00 | 0.00 | 1853.92 |
| 278 | 1971 | 1-(1H-pyrrol-2-yl)-ethanone | MS/RI | sweet, fruity, musty, cherry, nutty, wasabi, tea | 0.00 | 0.00 | 48.68 | 23.63 | 15.94 | 15.20 | 313.18 | 0.00 | 48.31 | 3943.20 | 125.62 | 42.31 | 53.32 | 4694.79 | 907.86 | 1410.90 | 1661.39 | 444.49 |
| 279 | 1971 | β-dihydroionol | MS/RI | woody, floral, amber | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 29.61 | 0.00 | 0.00 | 0.00 | 0.00 | 2667.22 |
| 280 | 1972 | (Z)-jasmone | MS/RI/S/O | woody, bitter, tea, with a citrus and floral nuance | 0.00 | 441.05 | 0.00 | 372.20 | 1303.26 | 2407.08 | 1141.35 | 88.03 | 5434.86 | 3864.04 | 1069.70 | 5924.99 | 792.13 | 834.95 | 805.90 | 615.68 | 733.15 | 14077.44 |
| 281 | 1972 | dodecanol | MS/RI | fat, soapy | 0.00 | 98.99 | 1287.76 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 282 | 1977 | 2H-pyran-2-one, tetrahydro-6-propyl- | MS/RI | coconut, sweet, creamy, lactonic and fruity | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 74.88 | 0.00 | 592.90 | 0.00 | 0.00 | 0.00 | 542.44 |
| 283 | 1992 | phenol | MS/RI | phenol，plastic | 344.58 | 82.77 | 175.93 | 434.66 | 0.00 | 80.38 | 99.79 | 40.99 | 103.25 | 772.72 | 124.67 | 196.20 | 129.22 | 970.67 | 312.78 | 448.19 | 874.16 | 596.05 |
| 284 | 2017 | trans-nerolidol | MS/RI/S/O | green, floral, woody, fruity, citrus, melon | 0.00 | 0.00 | 962.32 | 0.00 | 0.00 | 0.00 | 113.08 | 0.00 | 1297.37 | 37749.31 | 17922.78 | 61834.01 | 9415.46 | 6509.00 | 2678.10 | 4064.88 | 4044.98 | 31266.39 |
| 285 | 2021 | perilla alcohol | MS/RI | woody, cumin, spicy, cardamom, waxy, floral, oily, earthy | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 6.58 | 0.00 | 0.00 | 0.00 | 84.31 | 0.00 | 33.64 | 0.00 | 114.91 | 40.14 | 66.99 | 91.51 | 82.98 |
| 286 | 2028 | pyrrole-3-carboxaldehyde | MS/RI | musty, beefy, coffee | 151.27 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 2067.33 | 54.06 | 6.39 | 0.00 | 2717.67 | 364.08 | 2050.21 | 373.94 | 310.95 |
| 287 | 2032 | trans-cinnamaldehyde | MS/RI | sweet, spice, candy, cinnamon, red hots, warm | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 23.46 | 64.83 | 0.00 | 77.48 | 0.00 | 59.67 | 0.00 | 34.42 | 28.63 | 50.64 |
| 288 | 2034 | phenylethyl valerate | MS/RI | fruity, rose, leaf | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 27.39 | 23.25 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 399.81 | 105.32 | 0.00 | 193.86 | 293.08 |
| 289 | 2042 | dihydro-5-pentyl-2(3H)-furanone | MS/RI | coconut, peach | 36.94 | 0.00 | 0.00 | 12.71 | 0.00 | 36.07 | 38.55 | 0.00 | 0.00 | 1240.69 | 227.12 | 66.90 | 53.67 | 882.04 | 130.33 | 532.93 | 863.00 | 1194.82 |
| 290 | 2043 | furaneol | MS/RI/S/O | caramel | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 10.61 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 8.52 | 0.00 | 0.00 |
| 291 | 2049 | o-methoxybenzoic acid methyl ester | MS/RI | herbal, floral, hyacinth, fruity, blackcurrant | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 5.63 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 18.99 | 0.00 | 10.04 | 0.00 | 0.00 | 72.88 | 45.56 |
| 292 | 2050 | o-ethylphenol | MS/RI | phenolic | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 17.11 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 29.31 | 55.44 | 63.02 | 147.72 |
| 293 | 2050 | nerolidol | MS/RI/S | floral，green，waxy，citrus，woody | 271.10 | 0.00 | 162.53 | 17.30 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 194.36 | 116.27 | 796.51 | 0.00 | 188.51 | 0.00 | 0.00 | 0.00 | 559.86 |
| 294 | 2052 | 5-methyl-2-phenyl-2-hexenal | MS/RI | bitter cocoa, dark chocolate, aldehydic, coffee, nutty, honey, green | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 8.64 | 0.00 | 0.00 | 1297.75 | 0.00 | 0.00 | 0.00 | 176.78 | 1756.03 | 1580.99 | 1045.25 | 1065.79 |
| 295 | 2055 | diphenyl ether | MS/RI | rose, metallic | 172.49 | 22.54 | 149.06 | 35.42 | 24.76 | 176.10 | 141.28 | 26.47 | 272.83 | 213.22 | 0.00 | 52.48 | 51.72 | 134.96 | 231.71 | 269.05 | 388.96 | 285.83 |
| 296 | 2056 | hexyl benzoate | MS/RI | sweet, green, fruity, balsamic, orchid, metallic, cilantro | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 668.39 | 123.29 | 101.59 | 0.00 | 237.94 | 144.01 | 0.00 | 230.65 | 715.02 |
| 297 | 2057 | benzyl hexanoate | MS/RI | green, apricot, fruity, gardenia, jasmin | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 99.05 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 768.44 |
| 298 | 2058 | cuminic alcohol | MS/RI | wood, herb | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 170.08 | 0.00 | 61.96 | 152.63 | 0.00 | 30.62 | 259.12 | 271.46 | 301.82 |
| 299 | 2067 | 4-methylphenol | MS/RI | medicine, phenol, smoke | 0.00 | 0.00 | 21.05 | 51.15 | 0.00 | 8.49 | 22.65 | 0.00 | 0.00 | 637.26 | 11.51 | 0.00 | 0.00 | 657.38 | 174.51 | 273.58 | 480.09 | 474.29 |
| 300 | 2083 | octanoic acid | MS/RI | sweat, cheese | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 8.67 | 0.00 | 0.00 | 1028.16 | 28.01 | 26.24 | 0.00 | 449.48 | 132.84 | 406.04 | 1020.38 | 1154.84 |
| 301 | 2093 | cis-3-hexenyl benzoate | MS/RI | fatty, floral, green, fruity, spicy, woody | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 21.16 | 0.00 | 16.05 | 0.00 | 289.79 | 424.87 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 190.78 |
| 302 | 2103 | γ-decalactone | MS/RI | peach, fat | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 12.27 | 39.65 | 0.00 | 0.00 | 0.00 | 0.00 | 34.24 | 53.70 |
| 303 | 2106 | cedrol | MS/RI | woody, amber, floral, cedar, ambrette, musk | 1110.86 | 1309.43 | 0.00 | 0.00 | 13.07 | 89.71 | 121.73 | 26.42 | 748.47 | 0.00 | 0.00 | 0.00 | 0.00 | 84.76 | 1867.00 | 0.00 | 3038.87 | 0.00 |
| 304 | 2115 | m-cresol | MS/RI | fecal, plastic | 0.00 | 0.00 | 0.00 | 42.21 | 0.00 | 6.09 | 0.00 | 23.21 | 0.00 | 0.00 | 0.00 | 0.00 | 100.46 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 305 | 2153 | Thymol | MS/RI | phenolic, medicinal, woody, spicy | 0.00 | 36.35 | 0.00 | 0.00 | 0.00 | 223.18 | 3.79 | 0.00 | 0.00 | 160.24 | 19.62 | 383.13 | 0.00 | 0.00 | 92.13 | 823.85 | 153.39 | 0.00 |
| 306 | 2160 | 2-phenylethyl hexanoate | MS/RI | sweet, waxy, floral, fruity | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 172.02 | 0.00 | 447.08 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 307 | 2175 | τ-cadinol | MS/RI | balsam, earthy | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 59.18 | 0.00 | 14.92 | 0.00 | 0.00 | 62.07 | 0.00 | 0.00 | 0.00 | 181.33 | 883.59 | 298.06 | 0.00 |
| 308 | 2186 | 4-ethyl-phenol | MS/RI | phenolic, smoke, bacon and ham | 0.00 | 0.00 | 37.93 | 2.76 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 94.51 | 4.76 | 0.00 | 0.00 | 319.10 | 0.00 | 0.00 | 0.00 | 0.00 |
| 309 | 2188 | methyl 2-aminobenzoate | MS/RI | sweet, fruity, concord grape, with a musty and berry nuance | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 3.20 | 0.00 | 0.00 | 0.00 | 0.00 | 109.03 | 38.88 | 0.00 | 45.75 | 13.49 | 0.00 | 0.00 | 31.64 |
| 310 | 2189 | carvacrol | MS/RI | spicy, herbal, phenolic, medicinal, woody | 0.00 | 0.00 | 92.65 | 0.00 | 16.14 | 195.49 | 145.10 | 0.00 | 49.56 | 239.70 | 0.00 | 1097.66 | 1122.54 | 104.55 | 330.58 | 396.80 | 71.30 | 303.81 |
| 311 | 2190 | δ-amylvalerolactone | MS/RI | coconut, creamy, fatty, buttery, milky, nutty, fruity | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 857.13 | 663.17 | 836.55 | 125.93 | 307.68 | 0.00 | 68.95 | 92.39 | 1228.74 |
| 312 | 2202 | nonanoic acid | MS/RI | cheesy, fat | 96.00 | 0.00 | 134.65 | 0.00 | 0.00 | 38.70 | 39.68 | 0.00 | 17.04 | 1146.29 | 22.42 | 29.98 | 0.00 | 221.75 | 244.02 | 457.89 | 780.36 | 1214.09 |
| 313 | 2221 | α-cadinol | MS/RI | herb, wood | 0.00 | 23.75 | 0.00 | 0.00 | 0.00 | 38.41 | 45.94 | 30.97 | 21.38 | 120.84 | 288.93 | 60.67 | 0.00 | 0.00 | 346.92 | 2085.39 | 397.60 | 174.56 |
| 314 | 2273 | creamy lactone | MS/RI | creamy, fatty, coconut, peach and apricot | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 5.51 | 4541.90 | 3143.94 | 12746.83 | 2661.66 | 1893.83 | 77.35 | 152.77 | 240.63 | 8009.21 |
| 315 | 2325 | (2,6,6-trimethyl-2-hydroxycyclohexylidene)acetic acid lactone | MS/RI | fruity, apricot, woody, mango, berry, cherry, grape | 0.00 | 237.11 | 521.12 | 80.94 | 0.00 | 73.19 | 165.85 | 0.00 | 56.86 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 570.80 | 0.00 | 0.00 | 0.00 |
| 316 | 2332 | methyl jasmonate | MS/RI | floral, magnolia, fruity, green, jasmin, waxy, kiwi, melon | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 18.29 | 0.00 | 0.00 | 449.49 | 174.87 | 0.00 | 0.00 | 0.00 | 0.00 | 231.46 |
| 317 | 2350 | trans-farnesol | MS/RI | floral sweet | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 13.18 | 0.00 | 0.00 | 140.12 | 0.00 | 95.64 | 27.49 | 0.00 | 0.00 | 0.00 |
| 318 | 2441 | Indole | MS/RI/S/O | fecal, perfumey | 0.00 | 613.15 | 544.02 | 651.85 | 543.97 | 360.50 | 154.50 | 91.95 | 479.00 | 27578.99 | 0.00 | 39547.13 | 19184.91 | 5199.40 | 1222.19 | 2183.80 | 939.07 | 3594.80 |