

Effects of shaking and withering processes on the aroma qualities of black tea

Table S1. All volatile compounds detected by GC-MS/MS in the black teas processed under various conditions.

| NO | Name | RI ^a | RI ^b | Content (µg/L) | | | | | | | | | | | | | | | | | | | |
|----|---|-----------------|-----------------|----------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--|
| | | | | NS | WSR1F0 | WSR1F1 | WSR1F2 | WSR1F3 | WSR1F4 | WSR1F5 | WSR2F0 | WSR2F1 | WSR2F2 | WSR2F3 | WSR2F4 | WSR3F0 | WSR3F1 | WSR3F2 | WSR3F3 | WSR4F0 | WSR4F1 | WSR4F2 | |
| 1 | 2-Methylbutanal | 654.883 | 659 | 5.280 | 3.866 | 3.481 | 5.247 | 1.494 | 5.000 | 2.111 | 4.154 | 5.939 | 6.118 | 6.107 | 5.417 | 0.514 | 2.618 | 0.616 | 0.490 | 0.986 | 1.266 | 0.372 | |
| 2 | Hexanal | 795.242 | 800 | 2.830 | 4.796 | 6.169 | 6.593 | 7.175 | 8.300 | 8.200 | 3.683 | 4.885 | 6.631 | 8.325 | 9.165 | 5.018 | 5.598 | 5.290 | 9.485 | 12.677 | 9.410 | 6.007 | |
| 3 | trans-2-Hexenal | 847.000 | 850 | 0.311 | 5.560 | 11.751 | 8.240 | 10.637 | 8.418 | 8.551 | 6.655 | 9.325 | 11.597 | 9.511 | 7.912 | 3.867 | 13.222 | 11.328 | 14.699 | 16.171 | 11.397 | 11.919 | |
| 4 | Vanillin | 1003.433 | - | 1.015 | 1.385 | 0.676 | 0.854 | 0.777 | 0.630 | 0.656 | 0.822 | 0.316 | 0.673 | 0.447 | 0.818 | 0.356 | 0.620 | 1.338 | 1.390 | 0.321 | 0.532 | 1.023 | |
| 5 | Benzeneacetaldehyde | 1053.415 | 1049 | 28.628 | 11.030 | 27.330 | 10.574 | 19.952 | 27.075 | 32.022 | 9.801 | 28.788 | 21.543 | 26.532 | 31.439 | 1.542 | 1.925 | 2.650 | 3.902 | 3.818 | 3.889 | 27.607 | |
| 6 | 2,5-Dihydroxybenzaldehyde | 1127.359 | - | 3.112 | 5.176 | 2.519 | 3.547 | 3.410 | 2.022 | 1.547 | 3.077 | 2.022 | 2.970 | 2.668 | 3.406 | 1.144 | 2.299 | 2.837 | 3.333 | 3.665 | 2.592 | 1.965 | |
| 7 | 1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- | 1216.867 | 1214 | 1.441 | 2.025 | 2.245 | 2.610 | 2.671 | 2.377 | 2.577 | 1.917 | 2.162 | 3.022 | 2.857 | 2.719 | 1.005 | 3.104 | 2.110 | 2.951 | 3.394 | 2.062 | 1.837 | |
| 8 | Styrene | 902.986 | 890 | 0.204 | 0.015 | 0.172 | 0.009 | 0.143 | 0.062 | 0.060 | 0.102 | 0.013 | 0.242 | 0.407 | 0.015 | 0.022 | 0.125 | 0.019 | 0.088 | 0.136 | 0.073 | 0.025 | |
| 9 | β-Myrcene | 1006.568 | 992 | 27.833 | 21.353 | 21.555 | 19.955 | 20.111 | 13.236 | 13.466 | 16.069 | 19.943 | 15.913 | 15.728 | 18.553 | 8.473 | 13.450 | 21.897 | 12.469 | 18.907 | 11.917 | 17.271 | |
| 10 | D-Limonene | 1034.021 | 1029 | 4.152 | 3.392 | 3.537 | 2.813 | 3.212 | 2.300 | 1.829 | 2.499 | 3.131 | 2.428 | 2.820 | 2.779 | 0.903 | 2.117 | 3.230 | 2.224 | 2.832 | 2.067 | 2.530 | |
| 11 | β-Ocimene | 1057.149 | 1048 | 8.277 | 5.082 | 5.341 | 4.755 | 5.403 | 3.536 | 3.596 | 4.001 | 5.113 | 3.800 | 4.633 | 4.899 | 1.003 | 3.724 | 5.722 | 3.280 | 5.190 | 3.196 | 4.680 | |
| 12 | 3-Carene | 1022.247 | 1018 | 11.622 | 6.781 | 7.564 | 6.741 | 6.099 | 4.775 | 5.030 | 5.257 | 5.416 | 5.686 | 6.476 | 6.733 | 3.352 | 5.512 | 6.663 | 4.227 | 5.746 | 4.378 | 6.010 | |
| 13 | 4-Ethenyl-1,2-dimethyl-benzene | 1104.438 | - | 0.609 | 8.365 | 1.797 | 1.719 | 6.953 | 7.236 | 3.151 | 2.605 | 6.392 | 6.459 | 5.649 | 2.855 | 0.231 | 0.301 | 0.292 | 0.377 | 0.473 | 0.354 | 0.373 | |
| 14 | 1,5-Dimethyl-1,3-cyclohexadiene | 1189.792 | - | 8.575 | 1.643 | 1.510 | 1.386 | 0.761 | 0.620 | 0.878 | 0.851 | 0.830 | 0.997 | 1.077 | 0.723 | 0.213 | 1.793 | 7.543 | 7.911 | 5.375 | 2.299 | 5.561 | |
| 15 | Bicyclo[7.2.0]undec-4-ene,4,11,11-trimethyl-8-methylene-, (1R,4Z,9S)- | 1352.962 | - | 0.944 | 8.001 | 7.697 | 6.289 | 5.429 | 5.758 | 5.364 | 5.555 | 6.983 | 6.778 | 5.491 | 5.557 | 31.805 | 108.052 | 83.887 | 124.201 | 118.853 | 100.443 | 101.927 | |
| 16 | 4,7-Dimethyl-1-propan-2-yl-1,2,3,5,6,8a-hexahydronaphthalene | 1433.912 | - | 4.937 | 3.669 | 3.529 | 3.307 | 2.397 | 1.816 | 3.457 | 2.638 | 3.202 | 3.046 | 3.273 | 2.968 | 1.217 | 11.215 | 11.226 | 13.223 | 16.873 | 6.251 | 13.204 | |
| 17 | α-Calacorene | 1549.789 | 1546 | 4.121 | 0.607 | 0.335 | 0.443 | 0.798 | 0.714 | 0.787 | 0.664 | 0.760 | 0.342 | 0.525 | 0.489 | 3.292 | 4.978 | 5.109 | 5.083 | 5.428 | 4.211 | 4.832 | |
| 18 | (S)-(+)-3-Methyl-1-pentanol | 828.600 | - | 0.233 | 0.798 | 0.199 | 0.378 | 4.454 | 3.302 | 0.549 | 3.055 | 2.067 | 15.923 | 3.816 | 6.883 | 2.509 | 10.340 | 9.500 | 12.683 | 9.251 | 11.380 | 8.565 | |
| 19 | 3-Methyl-2-heptanol | 1038.201 | - | 2.216 | 0.004 | 0.745 | 0.011 | 0.071 | 1.439 | 1.200 | 0.650 | 0.611 | 0.232 | 1.468 | 0.927 | 0.143 | 2.490 | 0.240 | 0.280 | 0.682 | 0.177 | 0.156 | |
| 20 | Hydroxylamine, O-(diphenylmethyl)- | 1101.759 | - | 2.319 | 1.909 | 1.908 | 1.614 | 1.323 | 1.227 | 1.155 | 1.208 | 1.691 | 1.254 | 1.584 | 1.570 | 0.721 | 1.465 | 1.499 | 1.311 | 1.821 | 1.063 | 0.733 | |
| 21 | Linalool | 1111.691 | 1100 | 133.937 | 127.241 | 119.520 | 101.154 | 88.391 | 92.048 | 72.935 | 83.726 | 78.178 | 91.204 | 91.316 | 87.084 | 38.619 | 77.163 | 64.671 | 63.865 | 85.001 | 50.708 | 36.001 | |
| 22 | 3,7-Dimethyl-1,5,7-octatrien-3-ol | 1115.257 | 1108 | 86.726 | 55.103 | 45.368 | 50.814 | 34.082 | 48.998 | 36.974 | 38.685 | 37.102 | 22.400 | 63.686 | 46.163 | 37.105 | 26.931 | 29.022 | 34.835 | 47.822 | 25.951 | 15.487 | |
| 23 | (3R,6S)-2,2,6-Trimethyl-6-vinyltetrahydro-2H-pyran-3-ol | 1172.815 | 1183 | 12.673 | 9.017 | 9.664 | 11.142 | 8.849 | 10.331 | 9.498 | 9.936 | 9.334 | 9.379 | 12.382 | 13.325 | 1.186 | 13.632 | 14.652 | 13.942 | 13.655 | 11.919 | 11.139 | |
| 24 | α-Terpineol | 1183.828 | 1193 | 1.597 | 1.315 | 1.349 | 1.265 | 1.065 | 1.081 | 1.058 | 1.105 | 1.035 | 1.292 | 1.313 | 1.216 | 0.269 | 1.058 | 1.046 | 0.225 | 1.254 | 0.620 | 0.763 | |
| 25 | Geraniol | 1251.468 | 1257 | 341.232 | 262.717 | 240.466 | 259.121 | 207.200 | 228.265 | 231.352 | 215.484 | 204.859 | 266.268 | 246.829 | 254.265 | 260.169 | 251.332 | 168.633 | 216.046 | 279.394 | 136.637 | 130.037 | |
| 26 | 1,10-Di-epi-cubenol | 1613.827 | 1623 | 2.465 | 1.950 | 1.793 | 2.579 | 2.152 | 0.735 | 1.947 | 2.816 | 2.406 | 2.808 | 2.574 | 2.482 | 0.950 | 1.192 | 1.257 | 0.763 | 0.724 | 0.686 | 0.455 | |
| 27 | 2,6-Bis-tert-butyl-4-methylcyclohexanol | 1519.924 | - | 0.117 | 1.330 | 0.106 | 0.123 | 0.182 | 0.354 | 0.105 | 0.151 | 0.563 | 0.146 | 0.115 | 0.120 | 1.249 | 2.553 | 1.841 | 2.367 | 2.251 | 2.133 | 1.572 | |
| 28 | τ-Cadinol | 1635.190 | 1640 | 6.117 | 4.698 | 3.969 | 4.671 | 4.160 | 4.964 | 4.769 | 4.970 | 4.564 | 5.430 | 5.310 | 4.602 | 0.079 | 0.129 | 0.079 | 0.153 | 0.139 | 0.102 | 0.102 | |
| 29 | cis-3-Hexenyl acetate | 979.925 | - | 0.282 | 8.425 | 1.728 | 3.834 | 2.215 | 0.132 | 0.117 | 1.557 | 0.991 | 0.281 | 1.190 | 0.210 | 0.062 | 0.169 | 0.176 | 0.105 | 0.338 | 0.976 | 1.591 | |
| 30 | cis-5-Ethenyltetrahydro-α,α-5-trimethyl-2-furanmethanol | 1088.762 | 1078 | 27.448 | 21.515 | 21.608 | 17.800 | 14.446 | 15.758 | 11.808 | 15.293 | 18.002 | 13.742 | 18.185 | 18.192 | 7.751 | 15.624 | 15.720 | 13.728 | 17.217 | 8.625 | 7.311 | |
| 31 | Ethyl 2-(5-methyl-5-vinyltetrahydrofuran-2-yl)propan-2-yl carbonate | 1101.746 | 1090 | 89.200 | 75.477 | 71.477 | 59.340 | 50.248 | 47.899 | 41.996 | 50.290 | 61.731 | 59.696 | 59.708 | 57.756 | 28.288 | 58.616 | 56.672 | 51.230 | 64.129 | 31.504 | 29.227 | |
| 32 | 2-Propyn-1-ol,1-acetate | 1111.659 | - | 5.574 | 5.416 | 5.309 | 4.556 | 3.946 | 3.451 | 2.931 | 3.605 | 3.881 | 4.054 | 3.966 | 3.140 | 1.581 | 2.726 | 2.737 | 2.090 | 3.262 | 2.033 | 1.663 | |
| 33 | trans-Butanoic acid, 3-hexenyl ester | 1180.185 | - | 7.934 | 22.516 | 23.872 | 18.554 | 13.658 | 15.509 | 10.046 | 12.156 | 10.193 | 11.282 | 13.407 | 10.485 | 2.234 | 7.529 | 5.536 | 3.494 | 8.729 | 2.059 | 2.778 | |
| 34 | Methyl salicylate | 1187.015 | 1190 | 122.546 | 74.029 | 83.950 | 80.601 | 65.840 | 86.993 | 63.275 | 64.305 | 74.834 | 72.939 | 79.527 | 66.656 | 27.853 | 60.918 | 37.596 | 45.860 | 78.060 | 12.525 | 28.450 | |
| 35 | n-Valeric acid cis-3-hexenyl ester | 1222.118 | 1239 | 8.385 | 18.013 | 21.065 | 16.906 | 12.536 | 10.502 | 11.574 | 10.695 | 11.959 | 9.012 | 10.976 | 9.614 | 4.588 | 7.957 | 8.559 | 7.931 | 8.661 | 5.089 | 6.101 | |
| 36 | Butanedioic acid, bis(2-methylpropyl) ester | 1475.977 | - | 2.008 | 3.309 | 265.227 | 224.747 | 180.645 | 260.179 | 148.824 | 193.540 | 236.596 | 129.359 | 195.626 | 59.966 | 66.579 | 54.024 | 54.992 | 80.490 | 170.136 | 91.148 | 51.816 | |
| 37 | 2-Ethylhexyl acetate | 1148.916 | - | 0.060 | 0.321 | 0.365 | 0.383 | 0.325 | 0.579 | 0.302 | 0.281 | 0.122 | 0.147 | 0.218 | 0.136 | 0.043 | 0.214 | 0.109 | 0.140 | 0.096 | 0.134 | 0.153 | |
| 38 | trans-Geranic acid methyl ester | 1299.541 | 1321.7 | 0.246 | 0.710 | 0.908 | 0.730 | 0.700 | 0.568 | 0.515 | 0.596 | 0.528 | 0.179 | 0.664 | 0.316 | 0.171 | 0.473 | 0.028 | 0.374 | 0.510 | 0.226 | 0.157 | |
| 39 | cis-3-Hexenyl cis-hexanoate | 1329.136 | - | 26.082 | 100.349 | 104.852 | 97.818 | 61.338 | 60.770 | 62.912 | 66.123 | 59.809 | 59.532 | 69.301 | 58.196 | 22.187 | 54.145 | 47.687 | 35.478 | 41.876 | 29.592 | 33.418 | |

| | | | | | | | | | | | | | | | | | | | | | | |
|----|--|----------|--------|-------|-------|--------|--------|-------|--------|--------|-------|--------|--------|--------|-------|-------|-------|-------|-------|-------|-------|-------|
| 40 | Hexyl hexanoate | 1371.322 | 1385 | 2.132 | 7.024 | 7.010 | 6.966 | 3.300 | 3.843 | 4.349 | 3.989 | 3.413 | 4.893 | 5.766 | 3.595 | 1.428 | 3.492 | 1.643 | 2.247 | 3.336 | 2.114 | 1.882 |
| 41 | 2,2,6-Trimethylcyclohexanone | 1018.439 | 1022.9 | 1.441 | 0.226 | 0.289 | 0.317 | 0.260 | 0.298 | 0.296 | 0.219 | 0.328 | 0.262 | 0.258 | 0.422 | 0.174 | 0.265 | 0.325 | 0.215 | 0.444 | 0.252 | 0.236 |
| 42 | 4,7-Dimethyl-4,4a,5,6-tetrahydrocyclopenta[c]pyran-1,3-dione | 1210.361 | - | 1.688 | 0.838 | 1.020 | 1.035 | 0.798 | 1.026 | 0.969 | 0.731 | 0.884 | 1.109 | 1.170 | 1.054 | 0.267 | 0.832 | 0.950 | 0.612 | 0.967 | 0.584 | 0.597 |
| 43 | trans-8-Methyl-3,7-nonadien-2-one | 1225.402 | - | 0.648 | 0.497 | 2.616 | 0.717 | 0.367 | 0.762 | 0.633 | 6.535 | 0.601 | 0.629 | 0.809 | 0.804 | 0.016 | 1.009 | 0.683 | 0.824 | 1.004 | 0.685 | 0.476 |
| 44 | β-Ionone | 1476.623 | 1484 | 9.282 | 7.520 | 10.174 | 11.521 | 9.155 | 14.155 | 12.203 | 9.669 | 10.124 | 11.008 | 14.791 | 4.791 | 0.222 | 0.762 | 0.659 | 0.637 | 0.510 | 0.533 | 0.545 |
| 45 | 2-Ethylfuran | 750.514 | - | 1.703 | 1.669 | 1.650 | 3.285 | 2.749 | 3.695 | 2.130 | 2.234 | 1.702 | 3.410 | 4.015 | 4.089 | 3.160 | 3.418 | 3.395 | 3.318 | 4.079 | 2.335 | 0.485 |
| 46 | Toluene | 774.068 | - | 0.505 | 0.652 | 0.754 | 0.556 | 0.704 | 0.643 | 1.151 | 1.154 | 17.349 | 1.854 | 1.300 | 1.324 | 1.706 | 1.849 | 1.485 | 1.624 | 1.155 | 0.503 | 1.506 |
| 47 | Furfurylmethylamphetamine | 1026.202 | - | 1.863 | 2.335 | 2.957 | 3.188 | 2.643 | 3.209 | 2.505 | 2.257 | 2.028 | 3.061 | 3.583 | 3.961 | 2.808 | 2.703 | 3.041 | 3.427 | 3.590 | 3.032 | 0.993 |
| 48 | (1S,4S,4aS)-1-Isopropyl-4,7-dimethyl-1,2,3,4,4a,5-hexahydronaphthalene | 1300.372 | - | 1.109 | 2.212 | 2.333 | 2.220 | 1.931 | 1.857 | 1.701 | 1.914 | 2.137 | 2.478 | 1.879 | 1.819 | 1.203 | 2.071 | 1.953 | 1.903 | 2.497 | 1.343 | 1.476 |
| 49 | 1,2-Dihydro-4,5,7-trimethyl-naphthalene | 1303.274 | - | 0.663 | 0.388 | 0.448 | 0.497 | 0.271 | 0.158 | 0.462 | 0.276 | 0.223 | 0.245 | 0.566 | 0.178 | 0.147 | 0.154 | 0.205 | 0.193 | 0.158 | 0.091 | 0.077 |
| 50 | Hexanoic anhydride | 1336.192 | - | 2.509 | 6.082 | 7.206 | 6.804 | 3.221 | 3.595 | 3.622 | 5.145 | 3.076 | 4.053 | 4.908 | 2.645 | 0.505 | 2.509 | 2.571 | 2.405 | 2.882 | 2.786 | 2.369 |
| 51 | 2,4,6-Tri-tert-butylphenol | 1496.924 | - | 0.886 | 1.521 | 1.022 | 1.863 | 1.133 | 0.864 | 1.080 | 0.506 | 1.397 | 1.935 | 1.140 | 1.522 | 1.783 | 2.261 | 3.021 | 3.227 | 2.726 | 2.937 | 2.521 |

| NO | Name | RI ^a | RI ^b | Content (µg/L) | | | | | | | | | | | | | | | | | |
|----|---|-----------------|-----------------|----------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| | | | | SWR1F0 | SWR1F1 | SWR1F2 | SWR1F3 | SWR1F4 | SWR1F5 | SWR2F0 | SWR2F1 | SWR2F2 | SWR2F3 | SWR2F4 | SWR3F0 | SWR3F1 | SWR3F2 | SWR3F3 | SWR4F0 | SWR4F1 | SWR4F2 |
| 1 | 2-Methylbutanal | 654.883 | 659 | 2.231 | 0.374 | 0.358 | 0.426 | 0.931 | 1.715 | 2.846 | 1.528 | 0.663 | 4.116 | 2.798 | 0.557 | 4.731 | 4.447 | 3.084 | 1.479 | 0.403 | 0.103 |
| 2 | Hexanal | 795.242 | 800 | 0.896 | 1.872 | 2.074 | 3.235 | 1.813 | 1.974 | 2.895 | 0.933 | 2.839 | 2.944 | 4.197 | 1.925 | 3.093 | 2.376 | 5.690 | 4.098 | 2.053 | 6.374 |
| 3 | trans-2-Hexenal | 847.000 | 850 | 0.283 | 1.705 | 0.179 | 4.407 | 2.607 | 1.743 | 0.483 | 0.102 | 1.238 | 2.196 | 2.681 | 5.208 | 3.003 | 0.282 | 1.113 | 1.026 | 4.110 | 4.988 |
| 4 | Vanillin | 1003.433 | - | 1.539 | 1.727 | 0.801 | 1.110 | 0.967 | 1.365 | 1.585 | 0.984 | 0.877 | 0.363 | 1.082 | 1.523 | 1.442 | 1.541 | 1.153 | 1.085 | 1.228 | 1.416 |
| 5 | Benzeneacetaldehyde | 1053.415 | 1049 | 4.170 | 3.623 | 3.614 | 2.785 | 20.360 | 29.531 | 3.796 | 8.719 | 19.123 | 15.829 | 22.532 | 27.694 | 30.966 | 39.808 | 43.485 | 40.314 | 32.860 | 2.531 |
| 6 | 2,5-Dihydroxybenzaldehyde | 1127.359 | - | 3.188 | 2.191 | 2.470 | 1.667 | 2.211 | 3.763 | 3.821 | 1.193 | 4.144 | 3.560 | 2.454 | 3.817 | 3.193 | 3.192 | 2.975 | 2.903 | 2.593 | 1.959 |
| 7 | 1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- | 1216.867 | 1214 | 1.241 | 1.333 | 1.488 | 1.542 | 1.463 | 1.640 | 1.285 | 1.296 | 2.032 | 1.895 | 2.037 | 1.263 | 2.070 | 2.074 | 2.354 | 2.030 | 1.923 | 2.761 |
| 8 | Styrene | 902.986 | 890 | 0.049 | 0.179 | 0.022 | 0.012 | 0.049 | 0.073 | 0.027 | 0.013 | 0.031 | 0.189 | 0.053 | 0.039 | 0.059 | 0.018 | 0.479 | 0.187 | 0.070 | 0.060 |
| 9 | β-Myrcene | 1006.568 | 992 | 21.473 | 20.061 | 20.770 | 19.317 | 16.176 | 23.957 | 19.958 | 19.586 | 21.619 | 21.706 | 24.643 | 19.023 | 24.599 | 25.775 | 31.261 | 24.569 | 22.788 | 25.934 |
| 10 | D-Limonene | 1034.021 | 1029 | 3.616 | 3.290 | 3.352 | 3.215 | 3.249 | 3.814 | 2.740 | 2.872 | 2.409 | 3.402 | 3.972 | 3.120 | 3.924 | 4.113 | 4.574 | 3.671 | 3.260 | 4.017 |
| 11 | β-Ocimene | 1057.149 | 1048 | 6.585 | 5.505 | 5.673 | 5.396 | 3.748 | 6.914 | 5.264 | 5.146 | 6.359 | 6.074 | 7.106 | 5.290 | 7.433 | 8.573 | 9.153 | 6.569 | 6.172 | 7.917 |
| 12 | 3-Carene | 1022.247 | 1018 | 7.601 | 7.198 | 6.939 | 7.367 | 7.292 | 7.542 | 7.145 | 6.995 | 8.853 | 8.350 | 9.740 | 9.070 | 10.401 | 11.209 | 12.977 | 9.242 | 8.168 | 7.349 |
| 13 | 4-Ethenyl-1,2-dimethyl-benzene | 1104.438 | - | 0.525 | 0.451 | 0.507 | 0.337 | 0.548 | 0.449 | 0.196 | 0.435 | 0.486 | 0.435 | 0.644 | 0.512 | 0.486 | 0.609 | 0.520 | 0.576 | 0.422 | 0.481 |
| 14 | 1,5-Dimethyl-1,3-cyclohexadiene | 1189.792 | - | 8.094 | 3.724 | 5.632 | 2.130 | 4.031 | 4.926 | 5.220 | 1.456 | 10.088 | 7.546 | 6.489 | 3.638 | 8.341 | 4.127 | 2.921 | 4.453 | 7.777 | 9.508 |
| 15 | Bicyclo[7.2.0]undec-4-ene,4,11,11-trimethyl-8-methylene-, (1R,4Z,9S)- | 1352.962 | - | 100.000 | 121.210 | 100.000 | 95.327 | 97.472 | 87.477 | 100.000 | 93.068 | 94.282 | 97.444 | 100.568 | 97.406 | 91.747 | 81.964 | 103.318 | 94.228 | 91.400 | 96.777 |
| 16 | 4,7-Dimethyl-1-propan-2-yl-1,2,3,5,6,8a-hexahydronaphthalene | 1433.912 | - | 7.608 | 7.061 | 5.938 | 8.787 | 2.658 | 9.342 | 5.782 | 8.638 | 8.226 | 9.908 | 4.316 | 9.264 | 17.237 | 11.678 | 14.396 | 11.937 | 11.742 | 20.046 |
| 17 | α-Calacorene | 1549.789 | 1546 | 7.619 | 5.451 | 5.090 | 4.935 | 6.143 | 6.287 | 5.923 | 5.486 | 7.839 | 7.233 | 8.590 | 7.437 | 7.473 | 6.740 | 7.633 | 7.022 | 6.153 | 7.924 |
| 18 | (S)-(+)-3-Methyl-1-pentanol | 828.600 | - | 0.023 | 0.293 | 0.344 | 0.640 | 0.694 | 0.113 | 0.397 | 0.314 | 0.038 | 2.081 | 4.100 | 3.553 | 2.547 | 6.336 | 7.436 | 0.842 | 2.214 | 6.860 |
| 19 | 3-Methyl-2-heptanol | 1038.201 | - | 2.309 | 0.538 | 0.086 | 0.801 | 3.840 | 0.150 | 2.099 | 0.530 | 4.090 | 2.168 | 3.651 | 8.518 | 11.283 | 12.960 | 17.397 | 10.348 | 8.366 | 29.798 |
| 20 | Hydroxylamine, O-(diphenylmethyl)- | 1101.759 | - | 1.764 | 1.753 | 1.763 | 1.981 | 1.833 | 1.856 | 1.713 | 1.589 | 2.179 | 1.952 | 2.053 | 2.022 | 2.387 | 2.038 | 2.234 | 1.902 | 1.737 | 2.371 |
| 21 | Linalool | 1111.691 | 1100 | 118.305 | 112.610 | 109.694 | 93.954 | 120.479 | 111.080 | 123.763 | 97.079 | 149.770 | 116.069 | 114.085 | 93.513 | 127.218 | 105.630 | 103.780 | 99.344 | 87.792 | 86.222 |
| 22 | 3,7-Dimethyl-1,5,7-octatrien-3-ol | 1115.257 | 1108 | 32.365 | 39.641 | 45.658 | 31.157 | 43.184 | 42.935 | 40.416 | 32.268 | 54.891 | 70.236 | 56.977 | 31.031 | 82.557 | 44.983 | 34.919 | 34.132 | 24.044 | 49.234 |
| 23 | (3R,6S)-2,2,6-Trimethyl-6-vinyltetrahydro-2H-pyran-3-ol | 1172.815 | 1183 | 6.996 | 8.999 | 9.639 | 11.893 | 11.903 | 14.029 | 3.854 | 8.988 | 13.740 | 12.938 | 14.329 | 10.375 | 13.300 | 13.335 | 16.167 | 13.098 | 13.583 | 19.699 |
| 24 | α-Terpineol | 1183.828 | 1193 | 1.176 | 1.214 | 1.234 | 1.430 | 1.251 | 1.172 | 1.198 | 1.207 | 1.586 | 1.371 | 1.395 | 1.014 | 1.527 | 1.203 | 1.469 | 1.174 | 1.284 | 1.667 |
| 25 | Geraniol | 1251.468 | 1257 | 277.908 | 327.969 | 262.850 | 301.596 | 291.704 | 300.979 | 279.775 | 287.049 | 363.468 | 303.044 | 355.596 | 358.260 | 372.341 | 304.397 | 358.721 | 336.764 | 285.897 | 418.795 |
| 26 | 1,10-Di-epi-cubenol | 1613.827 | 1623 | 1.104 | 1.003 | 0.632 | 0.773 | 0.708 | 0.712 | 0.575 | 1.422 | 1.584 | 1.242 | 1.251 | 0.979 | 0.940 | 0.633 | 0.564 | 1.076 | 1.421 | 1.632 |
| 27 | 2,6-Bis-tert-butyl-4-methylcyclohexanol | 1519.924 | - | 2.163 | 3.062 | 2.728 | 1.946 | 1.871 | 2.545 | 2.765 | 2.629 | 3.445 | 2.961 | 2.719 | 2.090 | 2.795 | 2.630 | 1.086 | 2.784 | 2.131 | 2.871 |
| 28 | τ-Cadinol | 1635.190 | 1640 | 0.096 | 0.108 | 0.328 | 0.131 | 0.113 | 0.120 | 0.130 | 0.111 | 0.119 | 0.120 | 0.147 | 0.109 | 0.139 | 0.124 | 0.061 | 0.125 | 0.093 | 0.129 |
| 29 | cis-3-Hexenyl acetate | 979.925 | - | 0.692 | 1.739 | 0.168 | 1.793 | 0.186 | 0.165 | 1.035 | 1.567 | 0.201 | 0.250 | 0.218 | 0.395 | 0.458 | 0.295 | 0.257 | 0.227 | 0.177 | 0.459 |
| 30 | cis-5-Ethenyltetrahydro-α,α-5-trimethyl-2-furanmethanol | 1088.762 | 1078 | 21.942 | 21.405 | 22.188 | 23.660 | 24.425 | 22.929 | 19.314 | 17.308 | 25.115 | 22.735 | 24.140 | 17.054 | 26.980 | 23.246 | 24.248 | 21.980 | 18.590 | 26.115 |

| | | | | | | | | | | | | | | | | | | | | | |
|----|--|----------|--------|---------|---------|---------|---------|--------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 31 | Ethyl 2-(5-methyl-5-vinyltetrahydrofuran-2-yl)propan-2-yl carbonate | 1101.746 | 1090 | 68.362 | 67.802 | 68.053 | 75.213 | 80.444 | 73.337 | 66.714 | 59.691 | 94.093 | 75.671 | 80.894 | 58.824 | 91.238 | 79.742 | 90.692 | 84.541 | 66.447 | 93.720 |
| 32 | 2-Propyn-1-ol,1-acetate | 1111.659 | - | 5.250 | 4.850 | 4.911 | 5.059 | 5.198 | 4.188 | 4.018 | 3.075 | 6.566 | 5.109 | 4.913 | 3.914 | 5.980 | 4.325 | 4.417 | 4.253 | 4.111 | 2.563 |
| 33 | trans-Butanoic acid, 3-hexenyl ester | 1180.185 | - | 4.857 | 3.901 | 3.773 | 3.478 | 2.904 | 2.667 | 2.863 | 2.938 | 3.968 | 2.583 | 3.673 | 2.970 | 3.657 | 2.247 | 2.558 | 2.281 | 2.239 | 1.337 |
| 34 | Methyl salicylate | 1187.015 | 1190 | 61.583 | 79.862 | 70.089 | 67.489 | 73.877 | 97.067 | 91.992 | 77.775 | 72.512 | 89.070 | 104.411 | 77.837 | 108.776 | 76.039 | 100.932 | 66.534 | 75.293 | 95.248 |
| 35 | n-Valeric acid cis-3-hexenyl ester | 1222.118 | 1239 | 3.588 | 2.768 | 2.373 | 1.445 | 2.531 | 1.769 | 1.293 | 1.185 | 3.091 | 1.902 | 2.547 | 1.810 | 2.896 | 2.050 | 2.188 | 1.897 | 2.271 | 2.532 |
| 36 | Butanedioic acid, bis(2-methylpropyl) ester | 1475.977 | - | 109.701 | 186.745 | 169.485 | 167.732 | 41.217 | 107.695 | 134.409 | 103.282 | 179.318 | 183.815 | 162.145 | 139.352 | 178.097 | 130.373 | 140.791 | 102.167 | 51.822 | 63.675 |
| 37 | 2-Ethylhexyl acetate | 1148.916 | - | 0.149 | 0.072 | 0.095 | 0.083 | 0.150 | 0.155 | 0.110 | 0.086 | 0.157 | 0.154 | 0.086 | 0.120 | 0.149 | 0.120 | 0.079 | 0.085 | 0.083 | 0.160 |
| 38 | trans-Geranic acid methyl ester | 1299.541 | 1321.7 | 0.323 | 0.422 | 0.195 | 0.164 | 0.243 | 0.154 | 0.006 | 0.108 | 0.262 | 0.011 | 0.349 | 0.214 | 0.150 | 0.152 | 0.147 | 0.011 | 0.199 | 0.263 |
| 39 | cis-3-Hexenyl cis-hexanoate | 1329.136 | - | 27.996 | 19.994 | 15.920 | 10.514 | 11.473 | 13.450 | 12.806 | 13.504 | 20.298 | 16.892 | 23.507 | 19.812 | 22.681 | 16.155 | 13.838 | 14.704 | 19.885 | 21.137 |
| 40 | Hexyl hexanoate | 1371.322 | 1385 | 1.798 | 1.091 | 0.714 | 0.759 | 1.176 | 0.666 | 0.882 | 0.815 | 0.981 | 1.063 | 0.928 | 0.993 | 1.412 | 0.671 | 0.718 | 0.645 | 0.818 | 0.727 |
| 41 | 2,2,6-Trimethylcyclohexanone | 1018.439 | 1022.9 | 0.102 | 0.112 | 0.155 | 0.134 | 0.166 | 0.169 | 0.077 | 0.095 | 0.215 | 0.213 | 0.178 | 0.097 | 0.243 | 0.210 | 0.164 | 0.183 | 0.194 | 0.198 |
| 42 | 4,7-Dimethyl-4,4a,5,6-tetrahydrocyclopenta[c]pyran-1,3-dione | 1210.361 | - | 0.674 | 0.792 | 0.747 | 1.039 | 1.136 | 1.056 | 0.779 | 0.762 | 1.166 | 1.082 | 1.317 | 0.684 | 1.032 | 0.894 | 1.042 | 0.970 | 0.871 | 1.341 |
| 43 | trans-8-Methyl-3,7-nonadien-2-one | 1225.402 | - | 0.333 | 0.471 | 0.613 | 0.466 | 0.453 | 0.491 | 0.415 | 8.157 | 5.831 | 0.493 | 0.656 | 0.444 | 0.590 | 0.411 | 5.871 | 0.498 | 0.408 | 1.058 |
| 44 | β-Ionone | 1476.623 | 1484 | 1.442 | 0.800 | 0.765 | 0.863 | 1.109 | 0.958 | 0.868 | 1.100 | 1.618 | 1.239 | 1.586 | 1.410 | 1.125 | 0.840 | 0.750 | 1.166 | 1.354 | 0.614 |
| 45 | 2-Ethylfuran | 750.514 | - | 0.839 | 1.126 | 0.862 | 0.744 | 1.627 | 1.462 | 1.427 | 0.735 | 1.589 | 1.587 | 1.810 | 1.103 | 1.722 | 1.916 | 2.411 | 1.495 | 1.413 | 2.317 |
| 46 | Toluene | 774.068 | - | 0.569 | 0.972 | 0.639 | 0.935 | 1.718 | 1.347 | 1.006 | 4.789 | 2.478 | 0.619 | 1.076 | 1.148 | 1.252 | 1.338 | 1.697 | 0.997 | 1.229 | 1.150 |
| 47 | Furfurylmethylamphetamine | 1026.202 | - | 1.533 | 1.791 | 1.447 | 1.344 | 1.761 | 1.570 | 1.214 | 0.717 | 1.132 | 1.995 | 2.320 | 0.516 | 2.295 | 2.153 | 1.628 | 2.295 | 1.831 | 2.713 |
| 48 | (1S,4S,4aS)-1-Isopropyl-4,7-dimethyl-1,2,3,4,4a,5-hexahydronaphthalene | 1300.372 | - | 2.296 | 2.402 | 2.027 | 2.082 | 1.945 | 2.077 | 2.237 | 1.979 | 2.635 | 2.271 | 2.261 | 2.572 | 2.476 | 2.093 | 2.714 | 2.911 | 2.544 | 3.107 |
| 49 | 1,2-Dihydro-4,5,7-trimethyl-naphthalene | 1303.274 | - | 0.269 | 0.222 | 0.243 | 0.182 | 0.283 | 0.203 | 0.209 | 0.189 | 0.356 | 0.416 | 0.536 | 0.224 | 0.253 | 0.212 | 0.220 | 0.246 | 0.264 | 0.277 |
| 50 | Hexanoic anhydride | 1336.192 | - | 0.940 | 0.926 | 0.601 | 0.288 | 0.606 | 0.379 | 1.006 | 0.446 | 0.810 | 0.736 | 0.826 | 0.941 | 0.442 | 0.467 | 0.378 | 0.589 | 0.495 | 0.349 |
| 51 | 2,4,6-Tri-tert-butylphenol | 1496.924 | - | 3.987 | 3.446 | 2.357 | 2.648 | 3.228 | 3.686 | 3.230 | 3.437 | 4.130 | 4.465 | 4.970 | 3.987 | 4.042 | 3.838 | 3.579 | 3.809 | 3.755 | 2.983 |

Note: -: Not found yet. RI^a: The linear retention indices calculated from a series of n-alkanes (C7-C40). RI^b: Retention indices referred to the literature value with same or equivalent chromatographic column shown on NIST Chemistry WebBook (<http://webbook.nist.gov/chemistry/>).

Table S2. Volatile compounds responsible for aroma of the black teas and their odor activity values (OAVs) and odor characteristics.

| NO | Name | Odor Characteristics ^A | OTs (ug/L) ^B | OAVs | | | | | | | | | | | | | | | | | |
|----|---|-----------------------------------|-------------------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| | | | | WSR1F0 | WSR1F1 | WSR1F2 | WSR1F3 | WSR1F4 | WSR1F5 | WSR2F0 | WSR2F1 | WSR2F2 | WSR2F3 | WSR2F4 | WSR3F0 | WSR3F1 | WSR3F2 | WSR3F3 | WSR4F0 | WSR4F1 | WSR4F2 |
| 2 | Hexanal | Fresh, green, fruity | 4.5 | 1.066 | 1.371 | 1.465 | 1.595 | 1.845 | 1.822 | 0.818 | 1.085 | 1.474 | 1.850 | 2.037 | 1.115 | 1.244 | 1.176 | 2.108 | 2.817 | 2.091 | 1.335 |
| 3 | trans-2-Hexenal | Green banana | 17 | 0.327 | 0.691 | 0.485 | 0.626 | 0.495 | 0.503 | 0.391 | 0.549 | 0.682 | 0.559 | 0.465 | 0.227 | 0.778 | 0.666 | 0.865 | 0.951 | 0.670 | 0.701 |
| 6 | 2,5-Dihydroxybenzaldehyde | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 8 | Styrene | Sweet, balsam, floral | 730 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 9 | β-Myrcene | Sweet, citrus | 13.5 | 1.582 | 1.597 | 1.478 | 1.490 | 0.980 | 0.997 | 1.190 | 1.477 | 1.179 | 1.165 | 1.374 | 0.628 | 0.996 | 1.622 | 0.924 | 1.400 | 0.883 | 1.279 |
| 11 | β-Ocimene | Citrus, berbaceous, sweet | 34 | 0.149 | 0.157 | 0.140 | 0.159 | 0.104 | 0.106 | 0.118 | 0.150 | 0.112 | 0.136 | 0.144 | 0.030 | 0.110 | 0.168 | 0.096 | 0.153 | 0.094 | 0.138 |
| 12 | 3-Carene | Lemon, resin | 0.4 | 16.954 | 18.910 | 16.853 | 15.248 | 11.936 | 12.574 | 13.142 | 13.539 | 14.215 | 16.190 | 16.833 | 8.380 | 13.781 | 16.658 | 10.567 | 14.364 | 10.946 | 15.024 |
| 14 | 1,5-Dimethyl-1,3-cyclohexadiene | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 15 | Bicyclo[7.2.0]undec-4-ene,4,11,11-trimethyl-8-methylene-, (1R,4Z,9S)- | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 17 | α-Calacorene | Woody | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 20 | Hydroxylamine, O-(diphenylmethyl)- | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 25 | Geraniol | Mild, sweet rose fragrance | 40 | 6.568 | 6.012 | 6.478 | 5.180 | 5.707 | 5.784 | 5.387 | 5.121 | 6.657 | 6.171 | 6.357 | 6.542 | 6.283 | 4.216 | 5.401 | 6.985 | 3.416 | 3.251 |
| 27 | 2,6-Bis-tert-butyl-4-methylcyclohexanol | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 28 | τ-Cadinol | Tar, camphor and greasy | 0.44 | 10.677 | 9.021 | 10.616 | 9.455 | 11.282 | 10.840 | 11.294 | 10.373 | 12.341 | 12.067 | 10.459 | 0.179 | 0.293 | 0.180 | 0.349 | 0.315 | 0.232 | 0.232 |
| 30 | cis-5-Ethenyltetrahydro-α,α-5-trimethyl-2-furanmethanol | Floral, sweet, woody | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 31 | Ethyl 2-(5-methyl-5-vinyltetrahydrofuran-2-yl)propan-2-yl carbonate | Roasted, sweet | 320 | 0.236 | 0.223 | 0.185 | 0.157 | 0.150 | 0.131 | 0.157 | 0.193 | 0.187 | 0.187 | 0.180 | 0.088 | 0.183 | 0.177 | 0.160 | 0.200 | 0.098 | 0.091 |

| | | | | | | | | | | | | | | | | | | | | | |
|----|--------------------------------------|-----------------------------|-------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|---------|--------|---------|--------|--------|--------|--------|--------|
| 33 | trans-Butanoic acid, 3-hexenyl ester | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 35 | n-Valeric acid cis-3-hexenyl ester | Green, fruity | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 38 | trans-Geranic acid methyl ester | Green, fruity, flower | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 39 | cis-3-Hexenyl cis-hexanoate | Green, fruity | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 40 | Hexyl hexanoate | Sweet, fruity | 820 | 0.009 | 0.009 | 0.008 | 0.004 | 0.005 | 0.005 | 0.005 | 0.004 | 0.006 | 0.007 | 0.004 | 0.002 | 0.004 | 0.002 | 0.003 | 0.004 | 0.003 | 0.002 |
| 41 | 2,2,6-Trimethylcyclohexanone | Honey, cistus | 100 | 0.002 | 0.003 | 0.003 | 0.003 | 0.003 | 0.003 | 0.002 | 0.003 | 0.003 | 0.003 | 0.004 | 0.002 | 0.003 | 0.003 | 0.002 | 0.004 | 0.003 | 0.002 |
| 44 | β-Ionone | Woody and fruity | 0.007 | 1074.313 | 1453.406 | 1645.816 | 1307.892 | 2022.196 | 1743.251 | 1381.336 | 1446.323 | 1572.640 | 2112.980 | 684.361 | 31.739 | 108.926 | 94.072 | 90.944 | 72.800 | 76.150 | 77.878 |
| 45 | 2-Ethylfuran | Butter, caramel-like, burnt | 8000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.000 | 0.000 |
| 47 | Furfurylmethylamphetamine | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 50 | Hexanoic anhydride | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 51 | 2,4,6-Tri-tert-butylphenol | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

| NO | Name | Odor Characteristics ^A | OTs (ug/L) ^B | OAV | | | | | | | | | | | | | | | | | |
|----|---|-----------------------------------|-------------------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| | | | | SWR1F0 | SWR1F1 | SWR1F2 | SWR1F3 | SWR1F4 | SWR1F5 | SWR2F0 | SWR2F1 | SWR2F2 | SWR2F3 | SWR2F4 | SWR3F0 | SWR3F1 | SWR3F2 | SWR3F3 | SWR4F0 | SWR4F1 | SWR4F2 |
| 2 | Hexanal | Fresh, green, fruity | 4.5 | 0.199 | 0.416 | 0.461 | 0.719 | 0.403 | 0.439 | 0.643 | 0.207 | 0.631 | 0.654 | 0.933 | 0.428 | 0.687 | 0.528 | 1.264 | 0.911 | 0.456 | 1.416 |
| 3 | trans-2-Hexenal | Green banana | 17 | 0.017 | 0.100 | 0.011 | 0.259 | 0.153 | 0.103 | 0.028 | 0.006 | 0.073 | 0.129 | 0.158 | 0.306 | 0.177 | 0.017 | 0.065 | 0.060 | 0.242 | 0.293 |
| 6 | 2,5-Dihydroxybenzaldehyde | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 8 | Styrene | Sweet, balsam, floral | 730 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.000 | 0.000 | 0.000 |
| 9 | β-Myrcene | Sweet, citrus | 13.5 | 1.591 | 1.486 | 1.539 | 1.431 | 1.198 | 1.775 | 1.478 | 1.451 | 1.601 | 1.608 | 1.825 | 1.409 | 1.822 | 1.909 | 2.316 | 1.820 | 1.688 | 1.921 |
| 11 | β-Ocimene | Citrus, berbaceous, sweet | 34 | 0.194 | 0.162 | 0.167 | 0.159 | 0.110 | 0.203 | 0.155 | 0.151 | 0.187 | 0.179 | 0.209 | 0.156 | 0.219 | 0.252 | 0.269 | 0.193 | 0.182 | 0.233 |
| 12 | 3-Carene | Lemon, resin | 0.4 | 19.004 | 17.995 | 17.348 | 18.418 | 18.231 | 18.856 | 17.862 | 17.487 | 22.132 | 20.875 | 24.349 | 22.676 | 26.002 | 28.023 | 32.444 | 23.104 | 20.421 | 18.372 |
| 14 | 1,5-Dimethyl-1,3-cyclohexadiene | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 15 | Bicyclo[7.2.0]undec-4-ene,4,11,11-trimethyl-8-methylene-, (1R,4Z,9S)- | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 17 | α-Calacorene | Woody | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 20 | Hydroxylamine, O-(diphenylmethyl)- | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 25 | Geraniol | Mild, sweet rose fragrance | 40 | 6.948 | 8.199 | 6.571 | 7.540 | 7.293 | 7.524 | 6.994 | 7.176 | 9.087 | 7.576 | 8.890 | 8.956 | 9.309 | 7.610 | 8.968 | 8.419 | 7.147 | 10.470 |
| 27 | 2,6-Bis-tert-butyl-4-methylcyclohexanol | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 28 | τ-Cadinol | Tar, camphor and greasy | 0.44 | 0.219 | 0.245 | 0.194 | 0.298 | 0.257 | 0.272 | 0.295 | 0.252 | 0.270 | 0.272 | 0.333 | 0.248 | 0.317 | 0.282 | 0.138 | 0.284 | 0.742 | 0.293 |
| 30 | cis-5-Ethenyltetrahydro-α,α-5-trimethyl-2-furanmethanol | Floral, sweet, woody | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 31 | Ethyl 2-(5-methyl-5-vinyltetrahydrofuran-2-yl)propan-2-yl carbonate | Roasted, sweet | 320 | 0.214 | 0.212 | 0.213 | 0.235 | 0.251 | 0.229 | 0.208 | 0.187 | 0.294 | 0.236 | 0.253 | 0.184 | 0.285 | 0.249 | 0.283 | 0.264 | 0.208 | 0.293 |
| 33 | trans-Butanoic acid, 3-hexenyl ester | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 35 | n-Valeric acid cis-3-hexenyl ester | Green, fruity | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 38 | trans-Geranic acid methyl ester | Green, fruity, flower | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 39 | cis-3-Hexenyl cis-hexanoate | Green, fruity | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 40 | Hexyl hexanoate | Sweet, fruity | 820 | 0.002 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.002 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 |
| 41 | 2,2,6-Trimethylcyclohexanone | Honey, cistus | 100 | 0.001 | 0.001 | 0.002 | 0.001 | 0.002 | 0.002 | 0.001 | 0.001 | 0.002 | 0.002 | 0.002 | 0.001 | 0.002 | 0.002 | 0.002 | 0.002 | 0.002 | 0.002 |
| 44 | β-Ionone | Woody and fruity | 0.007 | 205.981 | 114.297 | 109.283 | 123.315 | 158.397 | 136.819 | 123.968 | 157.210 | 231.167 | 177.036 | 226.629 | 201.362 | 160.768 | 120.050 | 107.086 | 166.519 | 193.382 | 87.750 |
| 45 | 2-Ethylfuran | Butter, caramel-like, burnt | 8000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 47 | Furfurylmethylamphetamine | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 50 | Hexanoic anhydride | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 51 | 2,4,6-Tri-tert-butylphenol | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Note: OTs: Odor thresholds in water. The values were according to the reported references. A、B: (<http://www.thegoodscentscopy.com/search3.php?qOdor>; (Flaig, Qi, Wei, Yang, & Schieberle, 2020; Guo et al., 2021; H. Wang et al., 2020; M. Wang et al., 2020; Zhu et al., 2021; Zhu et al., 2018; Niu, Yao, Xiao, & Wu, 2016; Shu et al., 2016; Q., Zhang et al., 2019))