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**Fig. S1.** HPLC chromatogram of tea samples from Pingwu and other regions. PWT, Pingwu Fuzhuan brick tea (A); HNT, Hunan Fuzhuan brick tea (B); SNT, Shaanxi Fuzhuan brick tea (C); GZT, Guizhou Fuzhuan brick tea (D). Assigned peaks: 1, GA; 2, theobromine; 3, theophylline; 4, EGC; 5, C; 6, caffeine; 7, EGCG; 8, EC; 9, ECG.

**Table S1 Calibration for 27 mineral elements.**

|  |  |  |
| --- | --- | --- |
| Minerals | Regression | *R2* |
| Li | *y* = 23.157*x* + 29.004 | 0.998 |
| Be | *y* = 55.728*x* - 10.781 | 0.998 |
| Na | *y* = 596.46*x* + 50634 | 0.999 |
| Mg | *y* = 282.35*x* + 19105 | 0.999 |
| Al | *y* = 86.762*x* + 1220.2 | 0.999 |
| K | *y* = 214.06*x* + 29358 | 0.999 |
| Ca | *y* = 82.587*x* + 7291.2 | 0.999 |
| V | *y* = 6026.5*x* + 234.26 | 0.999 |
| Cr | *y* = 6998.5*x* + 3115.9 | 1 |
| Mn | *y* = 2797.6*x* + 8902.8 | 0.999 |
| Fe | *y* = 5848.2*x* + 37659 | 0.999 |
| Co | *y* = 13199*x* - 3565.3 | 0.999 |
| Ni | *y* = 4071.7*x* + 13099 | 0.999 |
| Cu | *y* = 10570*x* + 78811 | 0.999 |
| Zn | *y* = 1315.5*x* + 22742 | 0.999 |
| Ga | *y* = 2429.6*x* + 17731 | 0.999 |
| As | *y* = 997.28*x* + 74.587 | 1 |
| Se | *y* = 41.069*x* + 29.299 | 0.999 |
| Rb | *y* = 2205.5*x* + 52109 | 0.999 |
| Sr | *y* = 2933.4*x* + 21177 | 0.999 |
| Ag | *y* = 18781*x* - 1300.4 | 0.999 |
| Cd | *y* = 2222.3*x* + 13.495 | 1 |
| Cs | *y* = 9889.2*x* + 218.35 | 1 |
| Ba | *y* = 1806.2*x* + 18610 | 0.999 |
| Tl | *y* = 45279*x* + 333.36 | 1 |
| Pb | *y* = 29848*x* + 26059 | 1 |
| U | *y* = 64833*x* + 1199.2 | 1 |

**Table S2 Concentrations of 27 mineral elements of four regions FBTs. (μg/g)**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Elements | PWT | HNT | SNT | GZT |
| Li | 0.64 ± 0.01a | 0.42 ± 0.05a | 0.45 ± 0.02a | 0.29 ± 0.02a |
| Be | 0.04 ± 0.00a | 0.05 ± 0.01a | 0.04 ± 0.01c | 0.03 ± 0.00b |
| Na | 56.00 ± 0.64b | 35.83 ± 1.27a | 101.70 ± 2.69c | 97.50 ± 6.17c |
| Mg | 2303.35 ± 57.96bc | 1955.42 ± 154.61a | 2285.27 ± 60.29b | 2595.20 ± 123.03c |
| Al | 2530.56 ± 179.38b | 1541.07 ± 42.36a | 1460.44 ± 81.02a | 3074.22 ± 177.88c |
| K | 13467.76 ± 469.76a | 13339.03 ± 16.57a | 16809.47 ± 492.33b | 12535.76 ± 381.34a |
| Ca | 1108.74 ± 3.36c | 760.08 ± 84.12a | 718.02 ± 8.71a | 965.03 ± 26.99b |
| V | 0.73 ± 0.18b | 0.45 ± 0.01a | 0.49 ± 0.05a | 0.48 ± 0.04a |
| Cr | 1.81 ± 0.22a | 1.50 ± 0.06ab | 2.02 ± 0.22b | 1.59 ± 0.11a |
| Mn | 1265.26 ± 0.91b | 1530.97 ± 107.60c | 991.63 ± 8.26a | 2222.02 ± 57.84d |
| Fe | 565.17 ± 182.14b | 268.85 ± 33.22a | 315.31 ± 64.19ab | 255.08 ± 36.05a |
| Co | 0.50 ± 0.07b | 0.74 ± 0.06c | 0.34 ± 0.01a | 0.41 ± 0.02a |
| Ni | 6.05 ± 0.02b | 5.65 ± 0.44ab | 5.40 ± 0.23a | 6.18 ± 0.14b |
| Cu | 13.81 ± 0.15a | 17.97 ± 1.12c | 15.93 ± 0.41b | 16.55 ± 0.41b |
| Zn | 27.75 ± 0.22a | 27.38 ± 2.02a | 39.73 ± 1.69b | 26.90 ± 0.94a |
| Ga | 22.23 ± 0.52c | 17.03 ± 2.02b | 9.71 ± 1.58a | 23.03 ± 1.42c |
| As | 0.26 ± 0.02ab | 0.29 ± 0.03b | 0.25 ± 0.01a | 0.29 ± 0.03ab |
| Se | 0.18 ± 0.05a | 0.27 ± 0.02b | 0.22 ± 0.04ab | 0.25 ± 0.05ab |
| Rb | 47.38 ± 0.62a | 67.45 ± 3.07b | 80.82 ± 2.02c | 48.99 ± 0.92a |
| Sr | 40.17 ± 1.13d | 25.97 ± 2.12c | 19.50 ± 0.83b | 15.07 ± 0.30a |
| Ag | 0.01 ± 0.00a | 0.01 ± 0.00a | 0.01 ± 0.00a | 0.01 ± 0.00a |
| Cd | 0.08 ± 0.00ab | 0.09 ± 0.01b | 0.07 ± 0.01a | 0.10 ± 0.00c |
| Cs | 0.25 ± 0.02c | 0.21 ± 0.01b | 0.5 ± 0.02d | 0.16 ± 0.00a |
| Ba | 69.56 ± 1.40c | 47.81 ± 0.9b | 32.07 ± 1.57a | 67.17 ± 2.3c |
| Tl | 0.11 ± 0.01c | 0.07 ± 0.01b | 0.06 ± 0.000ab | 0.06 ± 0.00a |
| Pb | 1.95 ± 0.16b | 1.84 ± 0.08b | 1.13 ± 0.09a | 2.61 ± 0.14c |
| U | 0.02 ± 0.00a | 0.03 ± 0.00ab | 0.04 ± 0.01b | 0.03 ± 0.00ab |

All data were expressed as mean ± standard deviation (n = 3)

 a-d Means within each row with different letters are significantly different (*p* < 0.05).

**Table S3 Calibration, LOD, LOQ for GA, catechins and alkaloids.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| 　 | Regression | *R2* | LOD ng/mL | LOQ ng/mL |
| EGC | *y* = 3663812*x* + 15005 | 0.9999 | 105 | 319 |
| C | *y* = 15406343*x* + 41615 | 0.9998 | 35 | 105 |
| EGCG | *y* = 24307540*x* + 150895 | 0.9994 | 17 | 52 |
| EC | *y* = 17190611*x* + 177699 | 0.9997 | 215 | 652 |
| ECG | *y* = 35491455*x* + 128857 | 0.9994 | 12 | 36 |
| GA | *y* = 54696246*x* + 227742 | 0.9990 | 4 | 13 |
| theobromine | *y* = 106738749*x* + 84954 | 0.9994 | 4 | 13 |
| theophylline | *y* = 86330697*x* + 79214 | 0.9998 | 4 | 13 |
| caffeine | *y* = 61066523*x* + 415728  | 0.9991 | 7 | 23 |

**Table S4 Contents of volatile components in PWT, HNT, SNT and GZT (%)**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| No. | RT | Compounds | PWT | HNT | SNT | GZT |
| Volatile contents (%) |
|  |  | **Ketones** |  |  |  |  |
| 1 | 2.508 | 1-Penten-3-one | 0.87 ± 0.07 | - | 0.56 ± 0.54 | - |
| 2 | 9.139 | 2-Heptanone | 0.32 ± 0.02 | 0.31 ± 0.03 | 0.60 ± 0.03 | 0.45 ± 0.02 |
| 3 | 13.237 | 1-Hepten-3-one | 0.25 ± 0.04 | - | - | 0.16 ± 0.08 |
| 4 | 13.652 | 6-methyl-5-Hepten-2-one | 2.25 ± 0.11 | 2.72 ± 0.08 | 2.59 ± 0.10 | 3.73 ± 0.35 |
| 5 | 13.907 | 2-Pentyl furan | 2.05 ± 0.16 | 2.20 ± 0.08 | 3.13 ± 0.11 | 2.85 ± 0.44 |
| 6 | 14.33 | (E)-2-(2-Pentenyl)furan | - | - | 1.90 ± 0.05 | - |
| 7 | 16.012 | 2,2,6-trimethyl-Cyclohexanone | - | - | 0.75 ± 0.13 | - |
| 8 | 16.297 | 3-Octen-2-one | 0.15 ± 0.00 | 0.34 ± 0.06 | 0.28 ± 0.08 | 0.17 ± 0.12 |
| 9 | 17.535 | Acetophenone | - | 0.60 ± 0.23 | 0.40 ± 0.16 | 0.47 ± 0.28 |
| 10 | 17.862 | 3,5-Octadien-2-one | 3.56 ± 0.02 | 7.54 ± 0.16 | 5.52 ± 0.03 | 4.91 ± 0.40 |
| 11 | 18.243 | 3,4,4-Trimethyl-2-cyclohexen-1-one | - | 0.23 ± 0.08 | 0.42 ± 0.01 | - |
| 12 | 18.31 | 1,5-Cyclooctadien-4-one | 0.92 ± 0.02 | 0.33 ± 0.13 | - | - |
| 13 | 19.753 | 6-Methyl-3,5-heptadiene-2-one | - | - | 0.49 ± 0.08 | - |
| 14 | 20.601 | Isophorone | 0.19 ± 0.06 | 0.12 ± 0.01 | 0.13 ± 0.01 | 0.25 ± 0.16 |
| 15 | 21.933 | (E)-3-Nonen-2-one | 0.24 ± 0.00 | 0.44 ± 0.04 | 0.34 ± 0.05 | 0.62 ± 0.17 |
| 16 | 22.123 | (R,S)-5-Ethyl-6-methyl-3E-hepten-2-one | 0.44 ± 0.01 | 0.60 ± 0.07 | 0.61 ± 0.04 | 0.77 ± 0.10 |
| 17 | 24.627 | 1-(3-methylphenyl)-Ethanone | 0.33 ± 0.00 | 0.27 ± 0.04 | - | - |
| 18 | 25.3 | 2-Decanone | - | - | - | 0.21 ± 0.05 |
| 19 | 27.523 | 3-ethyl-4-methyl-1H-Pyrrole-2,5-dione | 0.19 ± 0.00 | 0.18 ± 0.04 | - | 0.11 ± 0.03 |
| 20 | 27.932 | 2,5-Octanedione | 0.10 ± 0.01 | 0.11 ± 0.01 | 0.19 ± 0.02 | 0.08 ± 0.01 |
| 21 | 29.695 | 1-(2,3,3-trimethyl-2-oxiranyl)-Ethanone | 0.23 ± 0.00 | 0.23 ± 0.02 | 0.27 ± 0.13 | 0.42 ± 0.05 |
| 22 | 29.941 | 3,4,4a,5,6,7-hexahydro-1,1,4a-trimethyl-2(1H)-Naphthalenone | 0.60 ± 0.01 | 0.33 ± 0.03 | - | 0.52 ± 0.08 |
| 23 | 33.894 | 2(3H)-Furanone, dihydro-5-pentyl- | 0.16 ± 0.00 | 0.12 ± 0.02 | 0.17 ± 0.06 | 0.10 ± 0.00 |
| 24 | 34.692 | 4-(2,4,4-Trimethyl-cyclohexa-1,5-dienyl)-but-3-en-2-one | 0.44 ± 0.01 | 0.33 ± 0.05 | 0.25 ± 0.05 | - |
| 25 | 36.859 | α-Ionone | 0.94 ± 0.03 | 0.91 ± 0.08 | 0.94 ± 0.11 | 0.84 ± 0.07 |
| 26 | 37.072 | 7-hydroxy-4-methyl-4-(propan-2-on-1-yl)-Tricyclo[3.3.0.0(2,8)]octan-3-one | 0.81 ± 0.03 | 0.88 ± 0.12 | 0.42 ± 0.04 | 0.27 ± 0.02 |
| 27 | 38.077 | 6,10-dimethyl-5,9-Undecadien-2-one, | 2.71 ± 0.12 | 2.06 ± 0.16 | 2.02 ± 0.14 | 3.08 ± 0.21 |
| 28 | 39.23 | 4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)but-3-en-2-one | 0.24 ± 0.00 | - | 0.26 ± 0.05 | - |
| 29 | 39.346 | (E)-β-Ionone | 1.26 ± 0.05 | 1.00 ± 0.07 | 1.08 ± 0.06 | 0.63 ± 0.03 |
| 30 | 39.449 | 4-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-3-Buten-2-one | 0.26 ± 0.02 | 0.23 ± 0.03 | 0.33 ± 0.03 | 0.16 ± 0.03 |
| 31 | 40.13 | 6,10-dimethyl-2-Undecanone | 0.14 ± 0.03 | 0.03 ± 0.01 | - | - |
| 32 | 40.671 | 3-Nonen-5-one | 0.33 ± 0.01 | 0.15 ± 0.05 | 0.26 ± 0.02 | - |
| 33 | 41.165 | 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-2(4H)-Benzofuranone | 0.56 ± 0.06 | 0.35 ± 0.08 | 0.63 ± 0.05 | 0.27 ± 0.02 |
| 34 | 41.374 | (E,Z)-6,10-dimethyl-3,5,9-Undecatrien-2-one | 0.10 ± 0.01 | - | - | 0.06 ± 0.00 |
| 35 | 42.587 | 2-Methyl-4-(1-methylethyl)-2-cyclohexenone | 0.29 ± 0.02 | 0.10 ± 0.01 | 0.17 ± 0.00 | 0.11 ± 0.01 |
| 36 | 43.62 | (E,E)- 6,10-dimethyl-3,5,9-Undecatrien-2-one | 0.08 ± 0.01 | 0.04 ± 0.01 | 0.07 ± 0.02 | 0.06 ± 0.01 |
| 37 | 47.737 | 2-Dodecanone | 0.08 ± 0.00 | 0.03 ± 0.01 | 0.06 ± 0.00 | 0.02 ± 0.00 |
| 38 | 50.604 | 6,10,14-trimethyl-2-Pentadecanone | 0.57 ± 0.02 | 0.49 ± 0.05 | 0.60 ± 0.06 | 0.35 ± 0.01 |
| 39 | 51.269 | Pentacosane-2,4-dione | - | 0.01 ± 0.00 | - | 0.01 ± 0.00 |
| 40 | 51.615 | (E,E)-6,10,14-trimethyl-5,9,13-Pentadecatrien-2-one | 0.05 ± 0.00 | 0.03 ± 0.00 | 0.03 ± 0.00 | 0.03 ± 0.01 |
|  |  | **Aldehydes** |  |  |  |  |
| 41 | 4.036 | (E)-2-Pentenal | 1.48 ± 0.03 | 0.34 ± 0.01 | - | 0.21 ± 0.04 |
| 42 | 5.476 | Hexanal | 5.58 ± 0.09 | 4.45 ± 0.50 | 2.02 ± 0.33 | 4.28 ± 0.35 |
| 43 | 6.613 | Furfural | 0.19 ± 0.09 | - | - | - |
| 44 | 7.513 | (E)-2-Hexenal | 1.47 ± 0.05 | 1.77 ± 0.23 | 0.66 ± 0.09 | 1.02 ± 0.07 |
| 45 | 12.191 | (Z)-2-Heptenal | - | 0.39 ± 0.02 | - | - |
| 46 | 12.345 | Benzaldehyde | 2.03 ± 0.01 | 2.24 ± 0.11 | 1.67 ± 0.08 | 1.65 ± 0.20 |
| 47 | 12.921 | 2-methyl-2-Heptenal | - | 1.42 ± 0.09 | 0.58 ± 0.08 | - |
| 48 | 14.236 | (E,E)-2,4-Heptadienal | 13.98 ± 0.13 | 13.22 ± 0.19 | 7.62 ± 0.31 | 11.38 ± 0.73 |
| 49 | 14.573 | Octanal | 2.23 ± 0.16 | 2.10 ± 0.22 | 1.82 ± 0.11 | 2.58 ± 0.30 |
| 50 | 16.454 | Phenylacetaldehyde | 0.27 ± 0.01 | 0.21 ± 0.05 | 0.27 ± 0.05 | - |
| 51 | 16.656 | 1-Ethyl-1H-pyrrole-2-carbaldehyde | 0.71 ± 0.04 | 0.95 ± 0.16 | 0.57 ± 0.03 | 0.29 ± 0.14 |
| 52 | 17.293 | (E)-2-Octenal | 3.59 ± 0.11 | 4.32 ± 0.24 | 1.80 ± 0.06 | 4.08 ± 0.24 |
| 53 | 19.823 | 1-Nonanal | 3.04 ± 0.34 | 3.10 ± 0.52 | 2.89 ± 0.23 | 4.42 ± 0.73 |
| 54 | 20.2 | 2,4-dimethyl-2,4-Heptadienal | - | - | - | 0.20 ± 0.01 |
| 55 | 20.746 | α-2-dimethyl-1-Cyclohexene-1-acetaldehyde | 0.06 ± 0.01 | 0.08 ± 0.01 | 0.13 ± 0.04 | 0.14 ± 0.06 |
| 56 | 22.806 | (E,Z)-2,6-Nonadienal | 0.64 ± 0.01 | 0.68 ± 0.10 | 0.37 ± 0.06 | 0.43 ± 0.20 |
| 57 | 23.287 | (E)-2-Nonenal | 1.49 ± 0.01 | 1.89 ± 0.22 | 1.11 ± 0.09 | 2.56 ± 0.30 |
| 58 | 24.043 | 2,4-Dimethylbenzaldehyde | 0.18 ± 0.01 | - | - | - |
| 59 | 25.497 | 2,6,6-trimethyl-1,3-Cyclohexadiene-1-carboxaldehyde | 0.47 ± 0.01 | 0.52 ± 0.04 | 0.85 ± 0.03 | 0.39 ± 0.08 |
| 60 | 26.12 | Decanal | 0.88 ± 0.00 | 1.13 ± 0.13 | 0.74 ± 0.06 | 1.28 ± 0.22 |
| 61 | 26.368 | 3,5-dimethyl-Benzaldehyde | 0.12 ± 0.01 | 0.23 ± 0.04 | 0.20 ± 0.05 | 0.19 ± 0.03 |
| 62 | 26.557 | (E,E)-2,4-Nonadienal | 0.22 ± 0.04 | 0.40 ± 0.04 | - | 0.51 ± 0.10 |
| 63 | 26.657 | 3,4-trimethyl-3-Cyclohexene-1-carboxaldehyde | 0.74 ± 0.05 | 0.86 ± 0.06 | 0.73 ± 0.04 | 0.74 ± 0.15 |
| 64 | 27.831 | (E)-Citral | 0.89 ± 0.04 | 0.32 ± 0.05 | - | 1.40 ± 0.17 |
| 65 | 31.566 | Undecanal | 0.22 ± 0.03 | - | - | 0.36 ± 0.05 |
| 66 | 32.008 | (E,E)-2,4-decadienal | 0.54 ± 0.01 | 0.53 ± 0.05 | 0.44 ± 0.07 | 0.63 ± 0.10 |
| 67 | 34.274 | 2-Undecenal | 0.26 ± 0.01 | 0.35 ± 0.04 | 0.16 ± 0.05 | 0.59 ± 0.12 |
| 68 | 38.903 | (E)-2-Dodecenal | 0.17 ± 0.01 | 0.12 ± 0.02 | 0.17 ± 0.02 | 0.12 ± 0.02 |
| 69 | 44.897 | Tridecanal | 0.04 ± 0.00 | 0.07 ± 0.03 | 0.03 ± 0.01 | 0.02 ± 0.00 |
|  |  | **Alcohols** |  |  |  |  |
| 70 | 4.282 | (z)-2-penten-1-ol | - | 0.50 ± 0.01 | 0.31 ± 0.00 | 0.43 ± 0.05 |
| 71 | 8.163 | 1-Hexanol | - | 0.21 ± 0.05 | 0.33 ± 0.03 | 0.31 ± 0.10 |
| 72 | 11.733 | 3-Ethyl-4-methylpentan-1-ol | - | 0.13 ± 0.02 | - | 0.16 ± 0.03 |
| 73 | 11.809 | 3-Nonen-1-ol | 0.19 ± 0.01 | - | 0.11 ± 0.02 | - |
| 74 | 13.005 | 1-Heptanol | 0.10 ± 0.01 | - | 1.33 ± 0.05 | 1.51 ± 0.47 |
| 75 | 13.487 | 1-Octen-3-ol | 0.37 ± 0.01 | 0.45 ± 0.04 | 0.50 ± 0.02 | 0.36 ± 0.09 |
| 76 | 15.923 | 2-Ethylhexanol | 1.60 ± 0.18 | 3.32 ± 0.41 | 1.32 ± 0.16 | 1.63 ± 0.09 |
| 77 | 18.027 | 1-Octanol | 0.72 ± 0.03 | 0.82 ± 0.05 | 0.79 ± 0.07 | 0.99 ± 0.18 |
| 78 | 19.579 | Linalool | 1.78 ± 0.08 | 2.18 ± 0.03 | 7.42 ± 0.28 | 4.16 ± 0.15 |
| 79 | 18.743 | (E)-Linalool oxide (furanoid) | 0.93 ± 0.16 | 2.51 ± 0.23 | 2.65 ± 0.10 | 2.89 ± 0.46 |
| 80 | 24.201 | (3R,6S)-2,2,6-Trimethyl-6-vinyltetrahydro-2H-pyran-3-ol | 0.54 ± 0.05 | 1.01 ± 0.34 | 1.34 ± 0.24 | 1.51 ± 0.56 |
| 81 | 25.354 | L-.alpha.-Terpineol | 0.72 ± 0.02 | 0.43 ± 0.07 | 0.90 ± 0.13 | 0.37 ± 0.07 |
| 82 | 25.607 | Thujyl alcohol | - | - | - | 0.14 ± 0.02 |
| 83 | 28.606 | 2,6-Octadien-1-ol, 2,7-dimethyl- | 0.45 ± 0.01 | 0.20 ± 0.02 | 0.44 ± 0.02 | 0.18 ± 0.02 |
| 84 | 30.834 | 4-Ethylcyclohexanol | 0.51 ± 0.03 | 0.48 ± 0.11 | 0.53 ± 0.04 | 0.70 ± 0.14 |
| 85 | 32.647 | 2,6,6-trimethyl-1-Cyclohexene-1-ethanol | - | 0.07 ± 0.01 | - | 0.03 ± 0.00 |
| 86 | 33.266 | 1-(1-Butyny)cyclopentanol | - | - | - | 0.05 ± 0.01 |
| 87 | 34.828 | 7-Tetradecanol | - | 0.16 ± 0.02 | 0.22 ± 0.04 | 0.27 ± 0.02 |
| 88 | 34.99 | cis-Hept-4-enol | 0.21 ± 0.02 | 0.10 ± 0.02 | 0.10 ± 0.02 | 0.11 ± 0.02 |
| 89 | 40.134 | 1-Heptacosanol | - | - | 0.17 ± 0.06 | - |
| 90 | 42.824 | Nerolidol | 1.29 ± 0.07 | - | 0.18 ± 0.02 | - |
| 91 | 43.122 | Phytol | 0.10 ± 0.00 | 0.12 ± 0.01 | 0.11 ± 0.02 | 0.10 ± 0.01 |
| 92 | 44.19 | Tridecanol | - | 0.03 ± 0.01 | 0.05 ± 0.01 | 0.03 ± 0.01 |
| 93 | 44.539 | (3R,3aS,6S,7R)-3,6,8,8-Tetramethyloctahydro-1H-3a,7-methanoazulen-6-ol | 0.90 ± 0.02 | 0.85 ± 0.15 | 0.75 ± 0.06 | 0.70 ± 0.09 |
| 94 | 48.501 | 2-hexyl-1-Decanol | 0.16 ± 0.01 | 0.14 ± 0.00 | 0.06 ± 0.02 | 0.12 ± 0.01 |
| 95 | 48.627 | 4,8-dimethyl-1-Nonanol | 0.03 ± 0.00 | 0.03 ± 0.01 | 0.04 ± 0.01 | 0.03 ± 0.00 |
| 96 | 50.438 | trans-Farnesol | 0.02 ± 0.00 | - | - | 0.02 ± 0.00 |
| 97 | 52.108 | Isophytol | 0.04 ± 0.00 | - | 0.01 ± 0.00 | - |
| 98 | 52.446 | (E)-3-Methyl-5-((1R,4aR,8aR)-5,5,8a-trimethyl-2-methylenedecahydronaphthalen-1-yl)pent-2-en-1-ol | 0.01 ± 0.00 | - | - | 0.01 ± 0.00 |
|  |  | **Esters** |  |  |  |  |
| 99 | 10.171 | Methyl N-hydroxybenzenecarboximidoate | - | - | - | 0.27 ± 0.02 |
| 100 | 10.697 | Methyl hexanoate | - | - | 0.04 ± 0.01 | 0.06 ± 0.01 |
| 101 | 25.075 | Methyl salicylate | 0.21 ± 0.01 | 0.85 ± 0.04 | 1.60 ± 1.22 | 0.81 ± 0.08 |
| 102 | 27.15 | Cyclopentaneundecanoic acid, methyl ester | 0.09 ± 0.01 | 0.08 ± 0.01 | 0.12 ± 0.00 | 0.11 ± 0.03 |
| 103 | 32.18 | 2,6-Octadienoic acid,3,7-dimethyl-, methyl ester | 0.09 ± 0.01 | 0.12 ± 0.03 | 0.14 ± 0.02 | 0.16 ± 0.01 |
| 104 | 33.351 | 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | 0.28 ± 0.00 | 0.36 ± 0.03 | 0.29 ± 0.02 | 0.24 ± 0.01 |
| 105 | 34.541 | 2-methyl-Propanoic acid-3-hydroxy-2,2,4-trimethylpentyl ester | 0.22 ± 0.00 | 0.22 ± 0.01 | 0.20 ± 0.08 | 0.18 ± 0.02 |
| 106 | 35.704 | Carbonic acid, decyl prop-1-en-2-yl ester | - | 0.03 ± 0.02 | 0.06 ± 0.04 | 0.05 ± 0.01 |
| 107 | 36.103 | Carbonic acid, nonyl prop-1-en-2-yl ester | 0.50 ± 0.03 | 0.44 ± 0.10 | 0.75 ± 0.05 | 0.66 ± 0.12 |
| 108 | 41.814 | Oxalic acid, 6-ethyloct-3-yl ethyl ester | - | - | - | 0.08 ± 0.02 |
| 109 | 50.328 | Isopropyl myristate | 0.36 ± 0.04 | 0.26 ± 0.18 | 0.19 ± 0.10 | 0.18 ± 0.21 |
| 110 | 50.842 | 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester | 0.03 ± 0.01 | 0.03 ± 0.01 | 0.03 ± 0.00 | 0.01 ± 0.00 |
| 111 | 51.823 | Hexadecanoic acid, methyl ester | 0.07 ± 0.00 | - | 0.03 ± 0.01 | 0.01 ± 0.00 |
| 112 | 52.69 | Hexadecanoic acid, ethyl ester | 0.02 ± 0.01 | 0.02 ± 0.01 | 0.02 ± 0.00 | 0.01 ± 0.00 |
|  |  | **Hydrocarbons** |  |  |  |  |
| 113 | 8.643 | 1-Ethyl-1,4-cyclohexadiene | - | - | 0.25 ± 0.03 | - |
| 114 | 11.052 | .alpha.-Pinene | - | - | 0.20 ± 0.15 | - |
| 115 | 13.09 | 3,5,5-Trimethyl-2-hexene | 0.16 ± 0.03 | - | - | - |
| 116 | 15.541 | 2-Methylenecyclohexanol | - | - | - | 0.26 ± 0.19 |
| 117 | 15.808 | Dipentene | - | - | 0.75 ± 0.14 | - |
| 118 | 17.025 | 1,1-Dimethyl-4-methylenecyclohexane | - | 0.72 ± 0.10 | 0.52 ± 0.04 | - |
| 119 | 20.103 | 3-(2-propenyl)-Cyclohexene | 0.82 ± 0.11 | 0.82 ± 0.12 | 1.04 ± 0.14 | 0.49 ± 0.06 |
| 120 | 21.256 | 2,11-Dodecanedione | 0.08 ± 0.00 | 0.22 ± 0.04 | 0.17 ± 0.03 | 0.36 ± 0.14 |
| 121 | 21.67 | 1-Methyl-1-(2-methyl-2-propenyl)cyclopentane | - | - | - | 0.21 ± 0.13 |
| 122 | 22.48 | 1,2-Dimethyl-4-ethylbenzene | - | 0.09 ± 0.04 | 0.21 ± 0.08 | 0.17 ± 0.16 |
| 123 | 24.457 | Azulene | 0.86 ± 0.07 | 1.35 ± 0.06 | 1.22 ± 0.04 | 1.31 ± 0.13 |
| 124 | 25.909 | 2,3,5,8-Tetramethyldecane | - | - | 0.15 ± 0.05 | 0.12 ± 0.03 |
| 125 | 27.302 | 5-methyl-1-Undecene | - | 0.18 ± 0.03 | 0.20 ± 0.05 | 0.37 ± 0.09 |
| 126 | 28.226 | 2,3-dihydro-4,7-dimethyl-1H-Indene | - | - | 0.12 ± 0.03 | 0.09 ± 0.02 |
| 127 | 28.852 | 1-methyl-4-(1-methyl-2-propenyl)-Benzene | 0.04 ± 0.01 | 0.07 ± 0.02 | 0.14 ± 0.01 | 0.06 ± 0.02 |
| 128 | 29.816 | 1,3-dimethyl-5-(1-methylethyl)-Benzene | 0.34 ± 0.04 | 0.25 ± 0.06 | 0.46 ± 0.03 | 0.38 ± 0.10 |
| 129 | 30.047 | 1-butenylidene-Cyclohexane | 0.58 ± 0.00 | 0.44 ± 0.05 | 0.23 ± 0.02 | 0.37 ± 0.09 |
| 130 | 30.616 | 1-methyl-Naphthalene | 2.11 ± 0.07 | 2.37 ± 0.30 | 2.10 ± 0.11 | 2.62 ± 0.44 |
| 131 | 31.213 | (E,Z)- 4,5-diethyl-3,5-Octadiene | 0.13 ± 0.01 | 0.10 ± 0.02 | - | 0.05 ± 0.00 |
| 132 | 31.634 | (1-methylheptyl)-Benzene | 0.19 ± 0.01 | 0.18 ± 0.05 | - | - |
| 133 | 32.334 | 3-Ethyl-3-methylheptane | - | 0.03 ± 0.01 | 0.10 ± 0.03 | 0.03 ± 0.00 |
| 134 | 32.904 | 8-methyl-1-Undecene | 0.19 ± 0.01 | 0.13 ± 0.02 | 0.19 ± 0.02 | 0.19 ± 0.02 |
| 135 | 33.574 | 1,2-dihydro-1,1,6-trimethyl-Naphthalene | 0.12 ± 0.01 | - | 0.05 ± 0.02 | - |
| 136 | 35.908 | 2,6-dimethyl-Naphthalene | 0.09 ± 0.02 | 0.06 ± 0.01 | 0.09 ± 0.02 | 0.08 ± 0.02 |
| 137 | 35.994 | 1,3-dimethyl-Naphthalene | 0.06 ± 0.01 | 0.16 ± 0.01 | - | 0.15 ± 0.03 |
| 138 | 36.411 | Dodecanal | 0.18 ± 0.01 | 0.30 ± 0.03 | 0.14 ± 0.01 | 0.26 ± 0.04 |
| 139 | 37.347 | cis-Thujopsene | 0.26 ± 0.01 | 0.23 ± 0.04 | 0.40 ± 0.06 | 0.24 ± 0.03 |
| 140 | 37.557 | 1-Dodecene | - | 0.04 ± 0.01 | 0.06 ± 0.00 | 0.05 ± 0.01 |
| 141 | 37.837 | 3,4,5,6-tetramethyl-2,5-Octadiene | - | 0.07 ± 0.01 | 0.09 ± 0.03 | 0.08 ± 0.00 |
| 142 | 38.333 | (E)-.beta.-Famesene | 0.09 ± 0.01 | - | - | - |
| 143 | 38.765 | 2,6,10-Trimethyl tridecane | 0.16 ± 0.01 | - | 0.25 ± 0.01 | 0.29 ± 0.06 |
| 144 | 39.722 | [4aR-(4a.alpha.,7.alpha.,8a.beta.)]-decahydro-4a-methyl-1-methylene-7-(1-methylethenyl)-Naphthalene | - | 0.05 ± 0.01 | 0.17 ± 0.01 | 0.07 ± 0.02 |
| 145 | 40.446 | Pentadecane | 0.36 ± 0.01 | 0.28 ± 0.08 | 0.39 ± 0.05 | 0.51 ± 0.07 |
| 146 | 40.531 | 1-(1,5-dimethyl-4-hexenyl)-4-methyl-Benzene | 0.25 ± 0.01 | 0.15 ± 0.04 | 0.28 ± 0.01 | 0.22 ± 0.03 |
| 147 | 40.895 | cis,cis-5,9-Tetradecadiene | - | - | 0.22 ± 0.00 | 0.33 ± 0.04 |
| 148 | 41.037 | [1S-(1.alpha.,4a.beta.,8a.alpha.)]-1,2,4a,5,8,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-Naphthalene | - | - | 0.08 ± 0.01 | - |
| 149 | 41.246 | (3E,7E)-4,8,12-Trimethyltrideca-1,3,7,11-tetraene | - | - | - | 0.08 ± 0.01 |
| 150 | 42.347 | 1-(Ethenesulfonyl)dodecane | - | - | - | 0.03 ± 0.01 |
| 151 | 42.427 | 6-methyl-Tridecane | - | - | - | 0.02 ± 0.01 |
| 152 | 42.513 | n-Nonylcyclohexane | - | - | - | 0.03 ± 0.01 |
| 153 | 43.047 | Hexadecane | 0.06 ± 0.00 | 0.04 ± 0.04 | 0.16 ± 0.02 | 0.07 ± 0.04 |
| 154 | 43.32 | 3-methyl-Pentadecane | 0.07 ± 0.00 | 0.04 ± 0.01 | 0.10 ± 0.02 | 0.06 ± 0.01 |
| 155 | 44.763 | 2,3,5,8-tetramethyl-Decane | 0.03 ± 0.01 | - | 0.02 ± 0.00 | 0.01 ± 0.00 |
| 156 | 45.467 | 1,2,3,4,4a,5,8,9,12,12a-decahydro-1,4-Methanobenzocyclodecene | 0.09 ± 0.01 | 0.07 ± 0.01 | 0.14 ± 0.04 | 0.05 ± 0.02 |
| 157 | 46.521 | 3-cyclohexyl-Undecane | 0.05 ± 0.01 | 0.06 ± 0.01 | 0.06 ± 0.00 | - |
| 158 | 46.627 | 4-methyl-Tetradecane | 0.02 ± 0.00 | 0.02 ± 0.01 | 0.04 ± 0.01 | 0.01 ± 0.00 |
| 159 | 46.833 | Octadecane | 0.04 ± 0.00 | 0.03 ± 0.01 | 0.07 ± 0.02 | 0.02 ± 0.01 |
| 160 | 46.938 | 2,2',5,5'-tetramethyl-1,1'-Biphenyl | 0.08 ± 0.00 | 0.06 ± 0.00 | 0.10 ± 0.01 | 0.06 ± 0.01 |
| 161 | 47.046 | 3,5,24-trimethyl-Tetracontane | - | - | 0.11 ± 0.03 | - |
| 162 | 47.266 | 3,4-diethyl-1,1'-Biphenyl | - | - | - | 0.03 ± 0.01 |
| 163 | 47.404 | 3-(2-cyclopentenyl)-2-methyl-1,1-diphenyl-1-Propene | - | - | - | 0.07 ± 0.01 |
| 164 | 47.93 | 2,6,10,14-tetramethyl-Pentadecane | 0.17 ± 0.02 | - | 0.16 ± 0.02 | 0.04 ± 0.01 |
| 165 | 48.845 | Hexacosane | 0.08 ± 0.00 | 0.05 ± 0.01 | 0.07 ± 0.02 | 0.04 ± 0.02 |
| 166 | 49.003 | Nonadecane | 0.03 ± 0.00 | 0.02 ± 0.01 | 0.03 ± 0.01 | 0.01 ± 0.00 |
| 167 | 49.136 | 11-(1-ethylpropyl)-Heneicosane | 0.03 ± 0.01 | 0.02 ± 0.01 | 0.02 ± 0.01 | 0.01 ± 0.00 |
| 168 | 49.816 | (E)-9-Eicosene | 0.02 ± 0.01 | 0.01 ± 0.00 | 0.01 ± 0.01 | 0.01 ± 0.00 |
| 169 | 49.943 | Tetracosane | 0.06 ± 0.01 | 0.05 ± 0.01 | 0.05 ± 0.00 | 0.04 ± 0.01 |
| 170 | 50.061 | 2,6,10,14-tetramethyl-Hexadecane | 0.09 ± 0.00 | 0.07 ± 0.01 | 0.07 ± 0.01 | 0.04 ± 0.01 |
| 171 | 50.206 | Tetradecanal | - | 0.01 ± 0.01 | - | - |
| 172 | 50.538 | Neophytadiene | 0.10 ± 0.01 | 0.05 ± 0.01 | 0.05 ± 0.01 | 0.02 ± 0.01 |
| 173 | 51.507 | 2-Methyl tetracosane | 0.01 ± 0.00 | - | 0.01 ± 0.00 | 0.04 ± 0.01 |
|  |  | **Phenol & Methoxyphenols** |  |  |  |  |
| 174 | 23.726 | 4-Ethylphenol | - | - | 0.25 ± 0.02 | - |
| 175 | 27.787 | 3,4-Dimethoxytoluene | - | - | 0.29 ± 0.04 | - |
| 176 | 31.535 | 1,2,3-Trimethoxybenzene | - | 0.59 ± 0.10 | 0.35 ± 0.01 | - |
| 177 | 32.12 | 4-ethyl-1,2-dimethoxy-Benzene | - | - | 0.10 ± 0.01 | - |
|  |  | **Acids** |  |  |  |  |
| 178 | 20.414 | 4-Ketopimelic acid | - | - | 0.12 ± 0.01 | - |
| 179 | 21.078 | 2-Ethyl-1-hexanoic acid | 0.12 ± 0.00 | - | 0.08 ± 0.02 | - |
| 180 | 24.84 | Octanoic acid | 0.33 ± 0.08 | 0.23 ± 0.07 | 0.22 ± 0.05 | 0.33 ± 0.25 |
| 181 | 52.264 | n-Hexadecanoic acid | - | - | 0.01 ± 0.01 | - |
|  |  | **Others** |  |  |  |  |
| 182 | 17.682 | 2-Acetyl pyrrole | 0.96 ± 0.32 | - | - | - |
| 183 | 21.439 | 1-Ethyl-2,5-pyrrolidinedione | 0.06 ± 0.00 | - | 0.16 ± 0.01 | 0.11 ± 0.03 |
| 184 | 28.75 | 3,5,6,8a-tetrahydro-2,5,5,8a-tetramethyl-2H-1-Benzopyran | - | - | 0.10 ± 0.02 | 0.06 ± 0.04 |
| 185 | 28.974 | 1-(1-oxobutyl)-Pyrrolidine | 0.01 ± 0.00 | 0.03 ± 0.02 | 0.06 ± 0.00 | - |
| 186 | 45.896 | N-[(pentafluorophenyl)methylene]-.β.,3,4-tris[(trimethylsilyl)oxy]-Benzeneethanamine | - | 0.08 ± 0.03 | 0.11 ± 0.05 | 0.07 ± 0.03 |
| 187 | 50.479 | Caffeine | 0.05 ± 0.00 | 0.08 ± 0.03 | 0.07 ± 0.02 | 0.04 ± 0.01 |
| 188 | 39.935 | 1-iodoHexadecane | 0.16 ± 0.01 | 0.07 ± 0.01 | 0.17 ± 0.01 | 0.14 ± 0.05 |

All data were expressed as mean ± standard deviation (n = 3). -, not detected.