

Table S1. Non-volatile compounds in roasted coffee examination by LC-MS.

| Non-volatile | Molecular formula | MW (g/mol) | t _R (min) | Area x10 ⁵ | | | | | |
|------------------|---|---------------|----------------------|-----------------------|---------------|-----------|------------------|----------------|------------------|
| | | | | OC | C | PM | LP | PM+LP | CC |
| Trigonelline | C ₇ H ₇ NO ₂ | 136.0404 | 8.40 | 4.130 | 7.160 | 5.530 | 6.950 | 5.210 | 5.920 |
| Chlorogenic acid | C ₁₆ H ₁₈ O ₉ | 353.0879 | 9.42 | 1,100.000 | 1,820.000 | 1,870.000 | 2,230.000 | 2,010.000 | 1,360.000 |
| Ferulic acid | C ₁₀ H ₁₀ O ₄ | 193.0505 | 11.93 | 6.690 | 7.790 | 7.240 | 8.310 | 5.560 | 7.880 |
| Quinic acid | C ₇ H ₁₂ O ₆ | 191.0561 | 1.38 | 2,280.000 | 2,280.000 | 1,870.000 | 2,010.000 | 1,780.000 | 2,300.000 |
| Malic acid | C ₄ H ₆ O ₅ | 133.0143 | 1.74 | 222.000 | 247.000 | 183.000 | 276.000 | 272.000 | 344.000 |
| Lactic acid | C ₃ H ₆ O ₃ | 89.02402 | 1.77 | 111.000 | 158.000 | 516.000 | 1,830.000 | 1,390.000 | 130.000 |
| Citric acid | C ₆ H ₈ O ₇ | 191.0198 | 1.92 | - | 16.000 | 0.558 | 53.400 | 31.900 | 181.000 |
| Tartaric acid | C ₄ H ₆ O ₆ | 149.0091 | 1.75 | 0.130 | 0.262 | - | 0.116 | 0.028 | 0.111 |
| Oxalic acid | C ₂ H ₂ O ₄ | 88.9876 | 1.74 | 14.800 | 7.960 | 12.300 | 12.200 | 12.700 | 13.700 |
| Citramalic acid | C ₅ H ₈ O ₅ | 147.0299 | 1.56 | 16.800 | 43.900 | 1.200 | 22.300 | 9.590 | 26.900 |
| Glutamic acid | C ₅ H ₉ NO ₄ | 146.0458 | 1.77 | 0.713 | 1.040 | 1.120 | 1.240 | 1.680 | 0.828 |
| Succinic acid | C ₄ H ₆ O ₄ | 117.0194 | 2.11 | 17.900 | 50.300 | 22.600 | 182.000 | 51.300 | 33.500 |
| Sucrose | C ₁₂ H ₂₂ O ₁₁ | 341.1089 | 1.39 | 38.100 | 36.700 | 19.600 | 29.900 | 19.000 | 45.900 |
| Fructose | C ₆ H ₁₂ O ₆ | 179.0561 | 1.55 | 139.000 | 45.500 | 93.800 | 50.900 | 41.900 | 108.000 |
| Catechins | C ₁₅ H ₁₄ O ₆ | 289.0719 | 10.79 | 3.660 | 8.820 | 5.720 | 9.210 | 5.800 | 6.840 |

Table S1. (continued)

| Non-volatile | Molecular formula | MW (g/mol) | t _R (min) | Area x10 ⁵ | | | | | |
|----------------------------|---|---------------|----------------------|-----------------------|---------------|---------------|---------------|---------------|--------------|
| | | | | OC | C | PM | LP | PM+LP | CC |
| Quercetin | C ₁₅ H ₁₀ O ₇ | 301.0354 | 1.46 | 0.106 | 0.166 | 0.127 | 0.165 | 0.304 | - |
| 1,3-Dicaffeoylquinic acid | C ₂₅ H ₂₄ O ₁₂ | 515.1196 | 11.97 | 2.340 | 11.900 | 0.457 | 7.650 | 8.380 | 8.150 |
| Niacin (Nicotinic acid) | C ₆ H ₅ NO ₂ | 122.0247 | 1.34 | 12.100 | 12.700 | 16.600 | 15.900 | 14.500 | 11.100 |
| Theophylline | C ₇ H ₈ N ₄ O ₂ | 179.0575 | 7.02 | 0.123 | 0.564 | 0.339 | 0.458 | 0.319 | 0.341 |
| Shikimic acid | C ₇ H ₁₀ O ₅ | 173.0454 | 1.42 | 33.200 | 16.800 | 18.600 | 43.100 | 40.900 | 18.300 |
| Beta-D-galacturonic acid | C ₆ H ₁₀ O ₇ | 193.0351 | 1.41 | 2.360 | 9.280 | 13.600 | 14.100 | 14.500 | 5.240 |
| 3-Hydroxyanthranilic acid | C ₇ H ₇ NO ₃ | 152.0353 | 9.29 | 21.300 | 42.600 | 71.200 | 54.400 | 47.600 | 23.200 |
| Chorismate | C ₁₀ H ₁₀ O ₆ | 225.0404 | 4.69 | 0.526 | 0.476 | 0.383 | 0.483 | 0.381 | 0.680 |
| Galactomannan | C ₁₈ H ₃₂ O ₁₆ | 503.1620 | 1.40 | 4.158 | 3.856 | 3.486 | 4.560 | 3.264 | 5.110 |
| <i>Cafeic acid pathway</i> | | | | | | | | | |
| L-Tyrosine | C ₉ H ₁₁ NO ₃ | 180.0667 | 11.84 | 2.290 | 4.940 | 3.080 | 5.710 | 4.990 | 5.230 |
| N-Hydroxy-L-tyrosine | C ₉ H ₁₁ NO ₄ | 197.0688 | 9.05 | 1.870 | 7.340 | 6.190 | 12.500 | 9.490 | 4.430 |
| 3-Coumaric acid | C ₉ H ₈ O ₃ | 164.0473 | 11.13 | 3.880 | 4.830 | 5.890 | 5.100 | 5.660 | 4.120 |
| Cafeic acid | C ₉ H ₈ O ₄ | 180.16 | 9.84 | 26.500 | 64.000 | 57.600 | 63.700 | 64.800 | 44.100 |

Table S1. (continued)

| Non-volatile | Molecular formula | MW (g/mol) | t _R (min) | Area x10 ⁵ | | | | | |
|--------------------|--|---------------|----------------------|-----------------------|--------------|-------|-------|-------|--------------|
| | | | | OC | C | PM | LP | PM+LP | CC |
| Caffeine pathway | | | | | | | | | |
| Xanthosine | C10H12N4O6 | 283.0672 | 1.42 | 0.119 | 0.699 | 0.201 | 1.130 | 0.622 | 0.445 |
| 7-Methylxanthosine | C11H15N4O6 | 298.0932 | 10.45 | 0.571 | 2.720 | 3.270 | 5.120 | 4.340 | 0.955 |
| 7-Methylxanthine | C6H6N4O2 | 165.0405 | 1.58 | 0.195 | 0.116 | 0.476 | 0.101 | 0.287 | 0.684 |
| Theobromine | C7H8N4O2 | 179.0574 | 7.02 | 0.081 | 0.564 | 0.227 | 0.458 | 0.319 | 0.236 |
| Caffeine | C ₈ H ₁₀ N ₄ O ₂ | 193.0731 | 1.42 | 1.700 | 1.620 | 0.339 | 0.741 | 0.491 | 1.610 |

Note: ordinary coffee (OC), control or non-fermentation (C; uninoculation), *P. motobuensis* JT-A29 (PM), *L. plantarum* JT-PN39 (LP), mixed starter cultures (PM+LP) fermented coffee and Civet coffee (CC).

Table S2. Volatile compounds in roasted coffee beans

| Compound | Aroma | Group | rt | Total peak area percentage (%) | | | | |
|---|--|----------------|--------|--------------------------------|---------------|---------------|---------------|---------------|
| | | | | OC | C | LP | PM+LP | PM |
| Acetic acid | sour | Acid | 1.978 | 31.42 | 31.49 | 59.92 | 20.63 | 4.95 |
| Butanoic acid | rancid butter, sour | Acid | 2.824 | 0.00 | 0.00 | 0.00 | 15.87 | 0.00 |
| Furfural | almond, nutty, sweet, caramel, bread | Furans | 3.399 | 33.49 | 44.01 | 68.37 | 59.76 | 64.14 |
| 2-Furanmethanol | caramellic, burnt, smoky | Alcohol | 3.667 | 100.00 | 100.00 | 78.23 | 100.00 | 100.00 |
| Pyrazine, 2,5-dimethyl- | coffee, cocoa, nutty, roasted, grassy | Pyrazine | 4.743 | 38.94 | 63.17 | 47.88 | 44.72 | 22.08 |
| 5-Methyl furfural | sweet, caramel, coffee | Furans | 5.946 | 55.91 | 54.92 | 100.00 | 59.66 | 66.13 |
| Pyrazine, 2-ethyl-6-methyl- | roasted, hazelnut-like | Pyrazine | 6.907 | 0.00 | 41.88 | 0.00 | 34.76 | 0.00 |
| 3,5-Dimethylcyclohex-1-ene-4-carboxaldehyde | floral | Aldehyde | 9.326 | 1.17 | 0.00 | 2.07 | 0.00 | 0.00 |
| Pyrazine, 2-ethyl-3,5-dimethyl- | wheat bread, smoked fatty fish, roast chicken, roast beef, black tea | Pyrazine | 9.499 | 6.15 | 13.72 | 7.50 | 5.38 | 11.96 |
| Maltol | caramel | Alcohol | 10.672 | 7.25 | 8.37 | 12.06 | 10.05 | 9.05 |
| 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- | caramel | Pyrans | 11.839 | 0.00 | 0.00 | 0.00 | 0.00 | 3.56 |
| Pyrazine, 3,5-diethyl-2-methyl- | green and nutty | Pyrazine | 12.483 | 0.00 | 6.14 | 0.00 | 0.00 | 0.00 |

Table S2. Volatile compounds in roasted coffee beans (continued)

| Compound | Aroma | Group | rt | Total peak area percentage (%) | | | | |
|--|---|----------|--------|--------------------------------|-------------|--------------|-------------|-------------|
| | | | | OC | C | LP | PM+LP | PM |
| 1H-Pyrrole, 1-(2-furanylmethyl)- | bread, roasted almond, popcorn, malt, roasted chicken, beer and sandalwood oil | Pyrrole | 13.506 | 3.05 | 3.24 | 2.66 | 4.29 | 1.79 |
| 2-Furancarboxaldehyde, 5- (hydroxymethyl)- | warm-herbaceous, winey-ethereal, hungarian chamomile, tobacco | Furans | 15.297 | 3.59 | 4.58 | 5.77 | 5.23 | 6.62 |
| 2-Cyclohexen-1-one, 4-(3-hydroxy-1- butenyl)-3,5,5-trimethyl-, [R-[R*,R*- (E)]]- | tobacco and tobacco smoke | Ketones | 16.108 | 0.49 | 0.86 | 0.98 | 1.20 | 1.21 |
| 2-Isoamyl-6-methylpyrazine | sour | Pyrazine | 16.232 | 0.00 | 3.89 | 1.97 | 0.00 | 1.21 |
| 10-Hydroxydecanoic acid | honey | Acid | 17.357 | 0.00 | 0.00 | 1.68 | 0.00 | 0.00 |
| Nonanoic acid | coconut | Acid | 17.657 | 0.86 | 0.92 | 0.21 | 0.51 | 0.10 |
| 4-Vinylguaiacol | clove, spicy | Phenols | 18.890 | 17.13 | 17.44 | 18.57 | 13.36 | 9.71 |
| Limonen-6-ol, pivalate | sweet, orange, citrus | Terpene | 19.305 | 0.00 | 0.00 | 0.37 | 0.00 | 0.13 |
| Tetradecane, 2,6,10-trimethyl- | fatty, dairy, coconut | Esters | 19.448 | 0.00 | 0.00 | 0.37 | 0.00 | 0.32 |
| Geranyl isovalerate | floral, fruity, apple | Phenols | 19.880 | 1.74 | 0.00 | 1.62 | 0.15 | 2.15 |

Table S2. Volatile compounds in roasted coffee beans (continued)

| Compound | Aroma | Group | rt | Total peak area percentage (%) | | | | |
|--|--|-----------|--------|--------------------------------|-------------|-------------|-------|------|
| | | | | OC | C | LP | PM+LP | PM |
| α -Furfuryliden- α -furylmethylamine | coffee-like, burnt aroma, sweet and spicy | Furans | 22.963 | 1.51 | 2.15 | 7.51 | 6.82 | 5.74 |
| 5-Methyl-2-phenyl-2-hexenal | cocoa, chocolate | Aldehydes | 26.058 | 0.00 | 0.62 | 0.67 | 0.00 | 0.58 |
| Megastigmatrienone | tobacco | Phenols | 29.451 | 0.13 | 0.13 | 0.16 | 0.13 | 0.00 |
| Hexadecane | gasoline | Alkane | 30.327 | 0.15 | 0.24 | 0.20 | 0.21 | 0.14 |

ordinary coffee (OC), control or non-fermentation (C; uninoculation), *P. motobuensis* JT-A29 (PM), *L. plantarum* JT-PN39 (LP) and mixed starter cultures (PM+LP) fermented coffee.