# Supplementary Information to

# Optimization of Fermentation Conditions and Metabolite Profiling of Grape Juice Fermented with Lactic Acid Bacteria for Improved Flavor and Bioactivity

*Part 1:Determination of the strains function and optimizing the fermentation conditions (Figure S1-S4; Table S1-S5)*

*Part 2: Analyses of metabolites profiles during the multi-strain fermentation stages (Figure S5-S7; Table S6-S8)*

*Part 3: Analyses of VOCs profiles (Figure S8; Table S8-S10)*

**Part 1:Determination of the strains function and optimizing the fermentation conditions (Figure S1-S4; Table S1-table S5)**

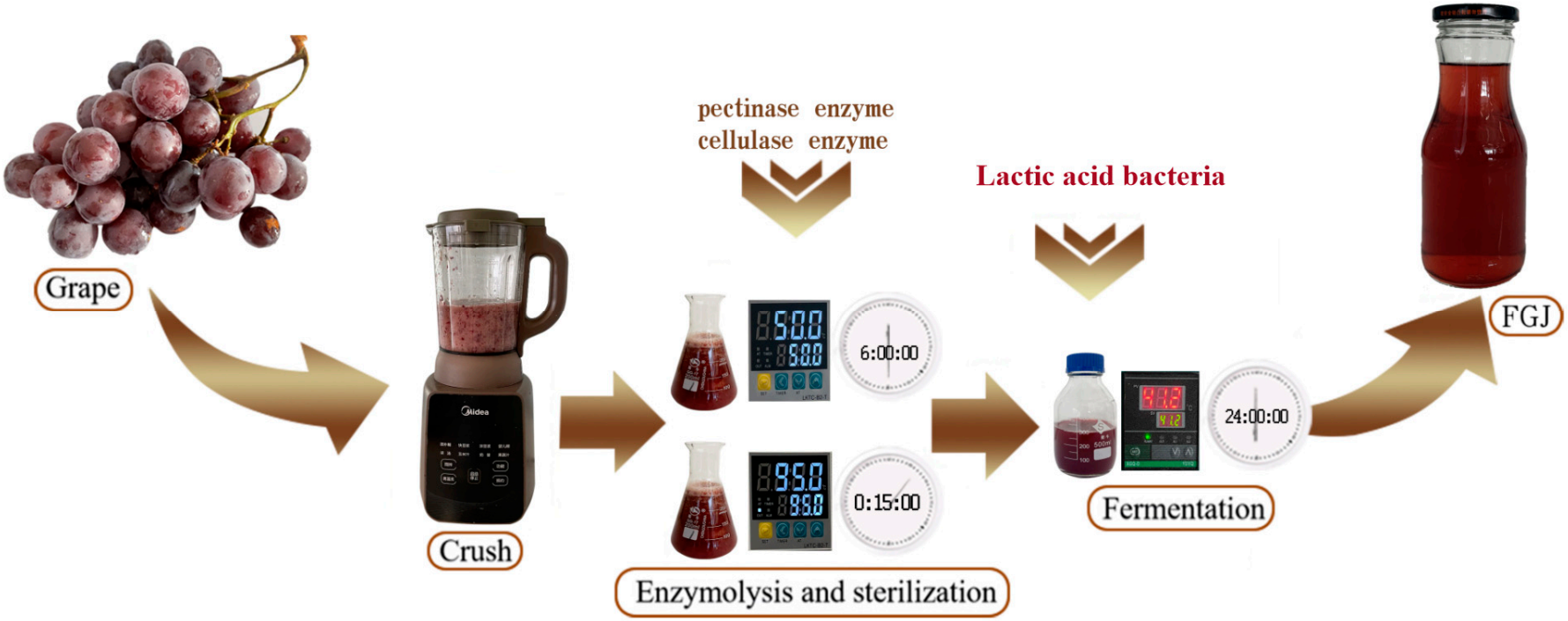


**Figure S1** The diagram of process flow of product FGJ

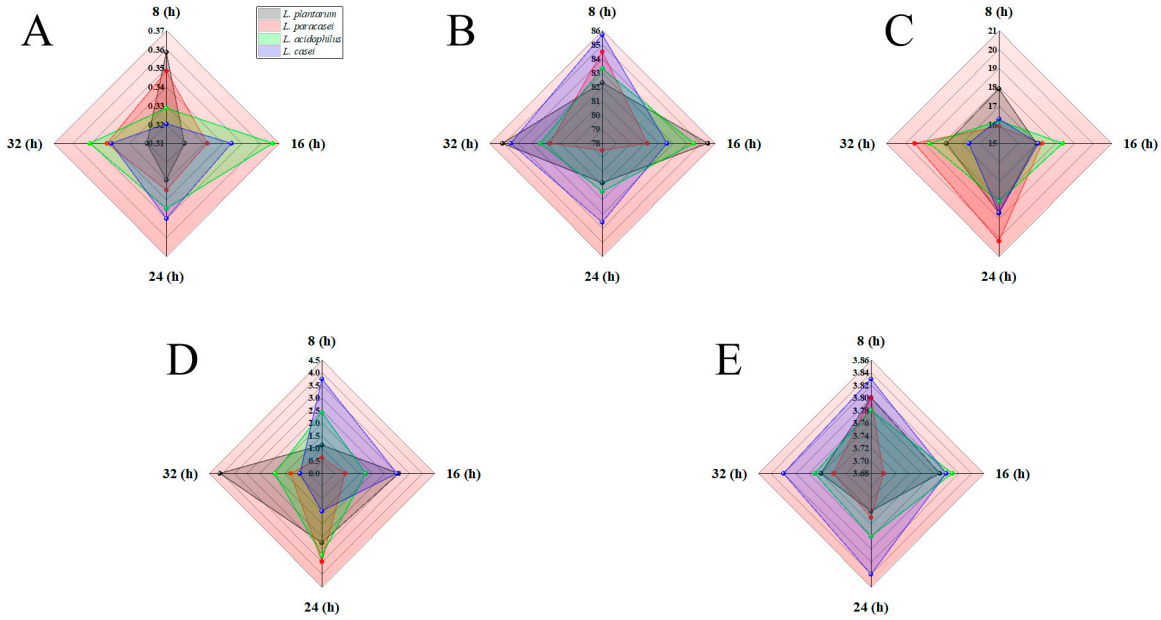


**Figure S2** Radar map analysis in TPC (A), clarification (B), TSS (C), LAB density (D), and pH (E) of FGJ during different single-strain (*L. plantarum, L. acidophilus, L. casei, L. paracasei*) fermentation stages

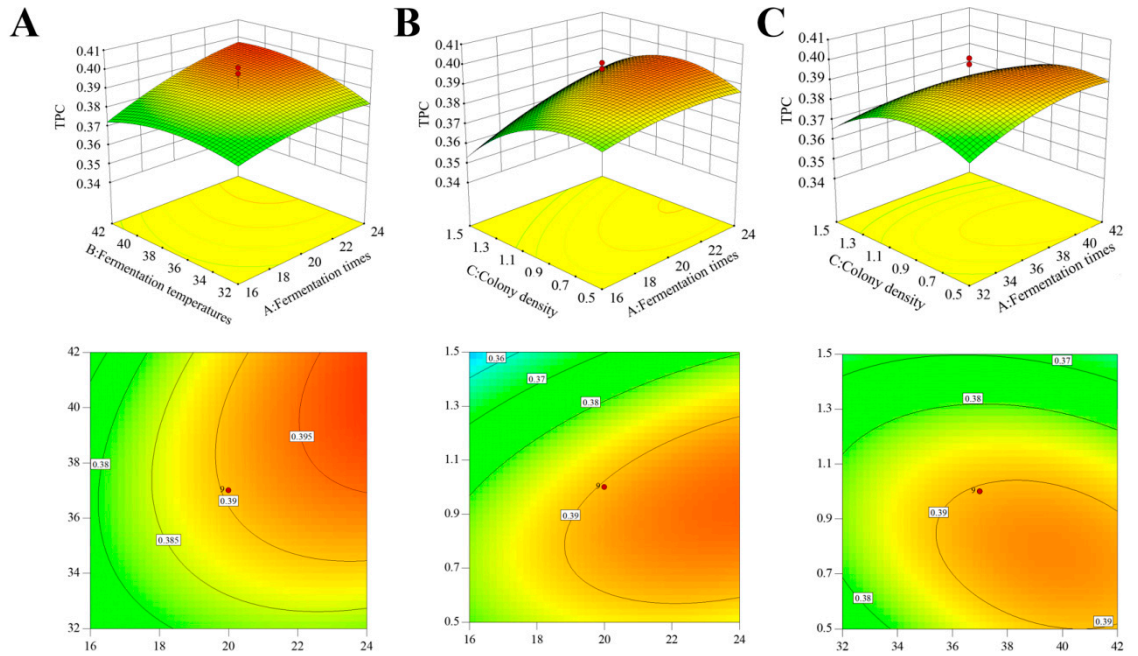


**Figure S3** Three-dimensional (3D) response surfaces of different factors (A:fermentation time; B:fermentation temperature; C:Colony density) on the TPC of FGJ

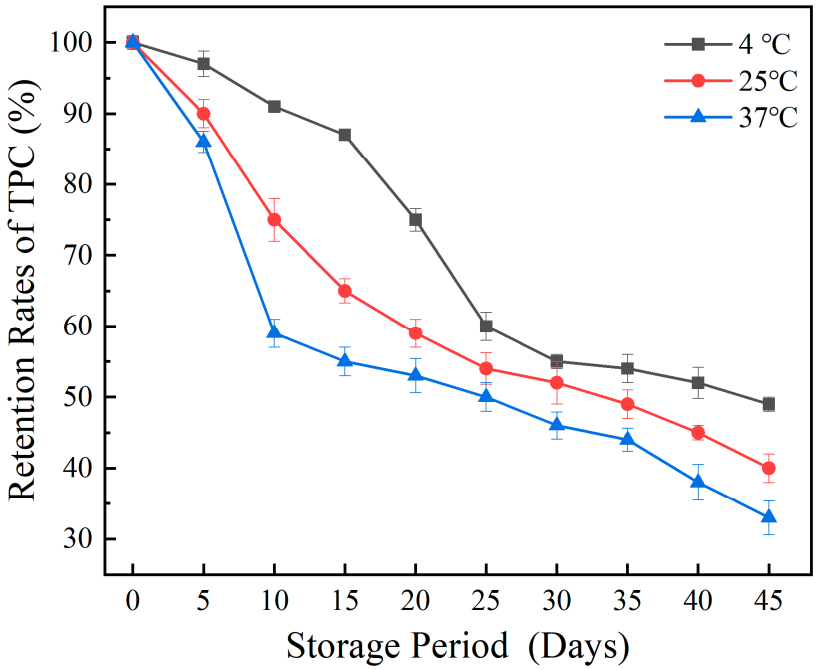


**Figure S4** Changes in retention rate of TPC during accelerated storage period

**Table S1** Uniform design factor level table

| Factor | *L. plantarum* X1/% | *L.acidophilus* X2/% | *L. case*i X3/% | *L. paracasei* X4/% |
|---|---|---|---|---|
| 1 | 0.64 | 0.61 | 0.55 | 0.43 |
| 2 | 0.65 | 0.65 | 0.58 | 0.46 |
| 3 | 0.67 | 0.62 | 0.56 | 0.47 |
| 4 | 0.63 | 0.66 | 0.52 | 0.48 |
| 5 | 0.66 | 0.64 | 0.51 | 0.41 |
| 6 | 0.62 | 0.67 | 0.57 | 0.42 |
| 7 | 0.68 | 0.68 | 0.54 | 0.44 |
| 8 | 0.61 | 0.63 | 0.53 | 0.45 |

**Table S2** Results of the uniform design experiment

| Factor | *L. plantarum* X1/% | *L.acidophilus* X2/% | *L. casei* X3/% | *L. paracasei* X4/% | TPC (mg GAE/mL) |
|---|---|---|---|---|---|
| 1 | 0.64 | 0.61 | 0.55 | 0.43 | 0.341 |
| 2 | 0.65 | 0.65 | 0.58 | 0.46 | 0.364 |
| 3 | 0.67 | 0.62 | 0.56 | 0.47 | 0.355 |
| 4 | 0.63 | 0.66 | 0.52 | 0.48 | 0.365 |
| 5 | 0.66 | 0.64 | 0.51 | 0.41 | 0.351 |
| 6 | 0.62 | 0.67 | 0.57 | 0.42 | 0.362 |
| 7 | 0.68 | 0.68 | 0.54 | 0.44 | 0.379 |
| 8 | 0.61 | 0.63 | 0.53 | 0.45 | 0.344 |

**Table S3** The level table of response surface factors

| Level | Factors | | |
|---|---|---|---|
| | A fermentation time (h) | B fermentation temperature (℃) | C LAB density ($10^7$CFU/mL) |
| -1.68 | 13.28 | 28.6 | 0.16 |
| -1 | 16 | 32 | 0.5 |
| 0 | 20 | 37 | 1 |
| 1 | 24 | 42 | 1.5 |
| 1.68 | 26.72 | 45.4 | 1.84 |

**Table S4** Experimental results of multi-strain fermentation by response surface design

| Number | A fermentation time (h) | B fermentation temperature (℃) | C LAB density ($10^7$ CFU/mL) | TPC (mg GAE/mL) |
|---|---|---|---|---|
| 1 | 16 | 32 | 1.5 | 0.348 |
| 2 | 26.73 | 37 | 1 | 0.392 |
| 3 | 24 | 32 | 0.5 | 0.367 |
| 4 | 16 | 32 | 0.5 | 0.373 |
| 5 | 20 | 37 | 1 | 0.386 |
| 6 | 20 | 37 | 1 | 0.385 |
| 7 | 16 | 42 | 1.5 | 0.345 |
| 8 | 20 | 37 | 1 | 0.389 |
| 9 | 20 | 45.41 | 1 | 0.377 |
| 10 | 24 | 32 | 1.5 | 0.373 |
| 11 | 20 | 37 | 1.84 | 0.343 |
| 12 | 24 | 42 | 0.5 | 0.399 |
| 13 | 16 | 42 | 0.5 | 0.378 |
| 14 | 20 | 37 | 1 | 0.387 |
| 15 | 20 | 37 | 1 | 0.388 |
| 16 | 13.27 | 37 | 1 | 0.370 |
| 17 | 20 | 28.59 | 1 | 0.374 |
| 18 | 20 | 37 | 0.16 | 0.370 |
| 19 | 24 | 42 | 1.5 | 0.377 |
| 20 | 20 | 37 | 1 | 0.401 |
| 21 | 20 | 37 | 1 | 0.398 |
| 22 | 20 | 37 | 1 | 0.390 |
| 23 | 20 | 37 | 1 | 0.390 |

**Table S5** Analysis of variance and significance test for the response values regression model

| Source of variance | Quadratic sum | Variance | Mean square | F Number | *p* Number | significance |
|---|---|---|---|---|---|---|
| Model | 0.00544 | 9 | 0.00060 | 21.65 | < 0.0001 | ** |
| A-Fermentation time | 0.00087 | 1 | 0.00087 | 31.19 | < 0.0001 | ** |
| B-Fermentation | 0.00014 | 1 | 0.00014 | 4.86 | 0.0460 | * |
| C-temperature | 0.00104 | 1 | 0.00104 | 37.43 | < 0.0001 | ** |
| AB | 0.00014 | 1 | 0.00014 | 5.18 | 0.0404 | * |
| AC | 0.00022 | 1 | 0.00022 | 7.90 | 0.0147 | * |
| BC | 0.00016 | 1 | 0.00016 | 5.81 | 0.0315 | * |
| A2 | 0.00017 | 1 | 0.00017 | 6.21 | 0.0270 | * |
| B2 | 0.00044 | 1 | 0.00044 | 15.68 | 0.0016 | ** |
| C2 | 0.00227 | 1 | 0.00227 | 81.53 | < 0.0001 | ** |
| Residual | 0.00036 | 13 | 0.00003 | | | |
| Unplanned item | 0.00012 | 5 | 0.00002 | 0.84 | 0.5594 | Not significant |
| Error term | 0.00024 | 8 | 0.00003 | | | |
| Total | 0.00580 | 22 | | | | |
| $R^2$=0.9386 | $R^2$Adj=0.8960 | | | | | |

**Part 2: Analyses of metabolites profiles during the multi-strain fermentation stages (Figure S5-S7; Table S6-S8)**

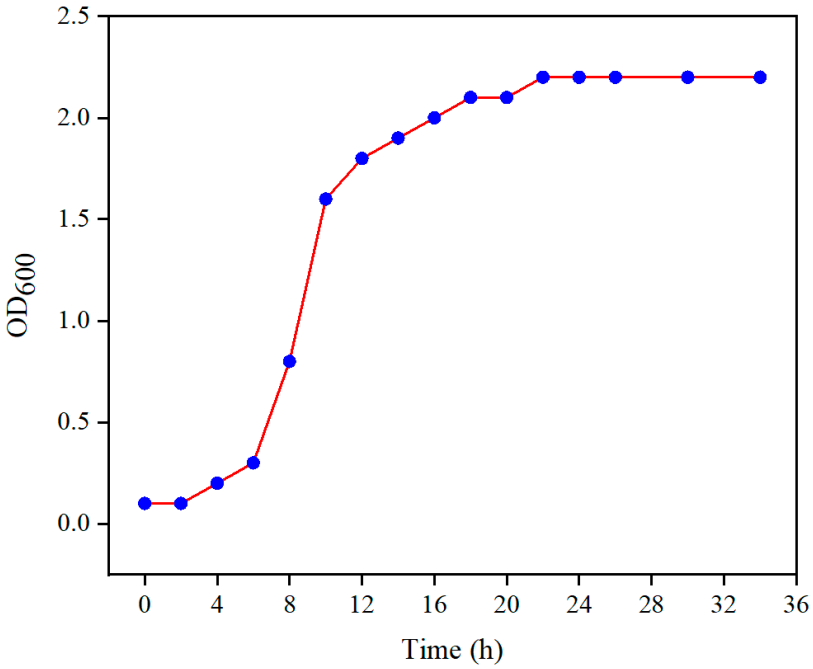


**Figure S5** Growth curve analysis of multi-strain during different incubate stages

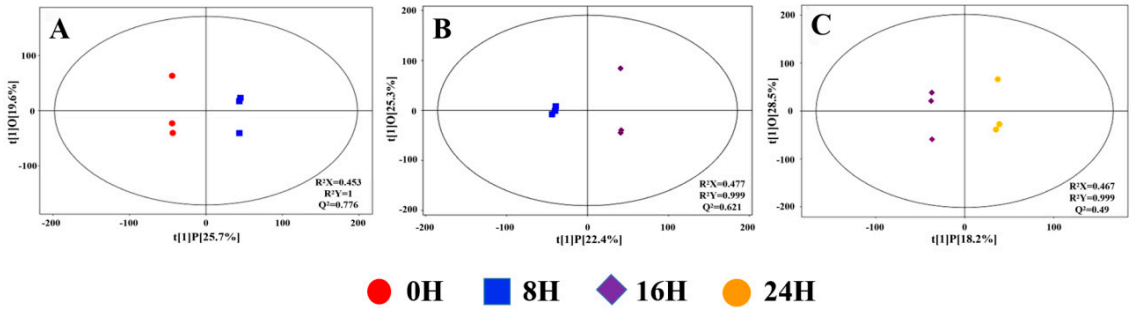


**Figure S6** OPLS-DA score plots analysis of FGJ during different multi-strain fermentation stages (A: 0-8h; B: 8-16h; C:16-24h)

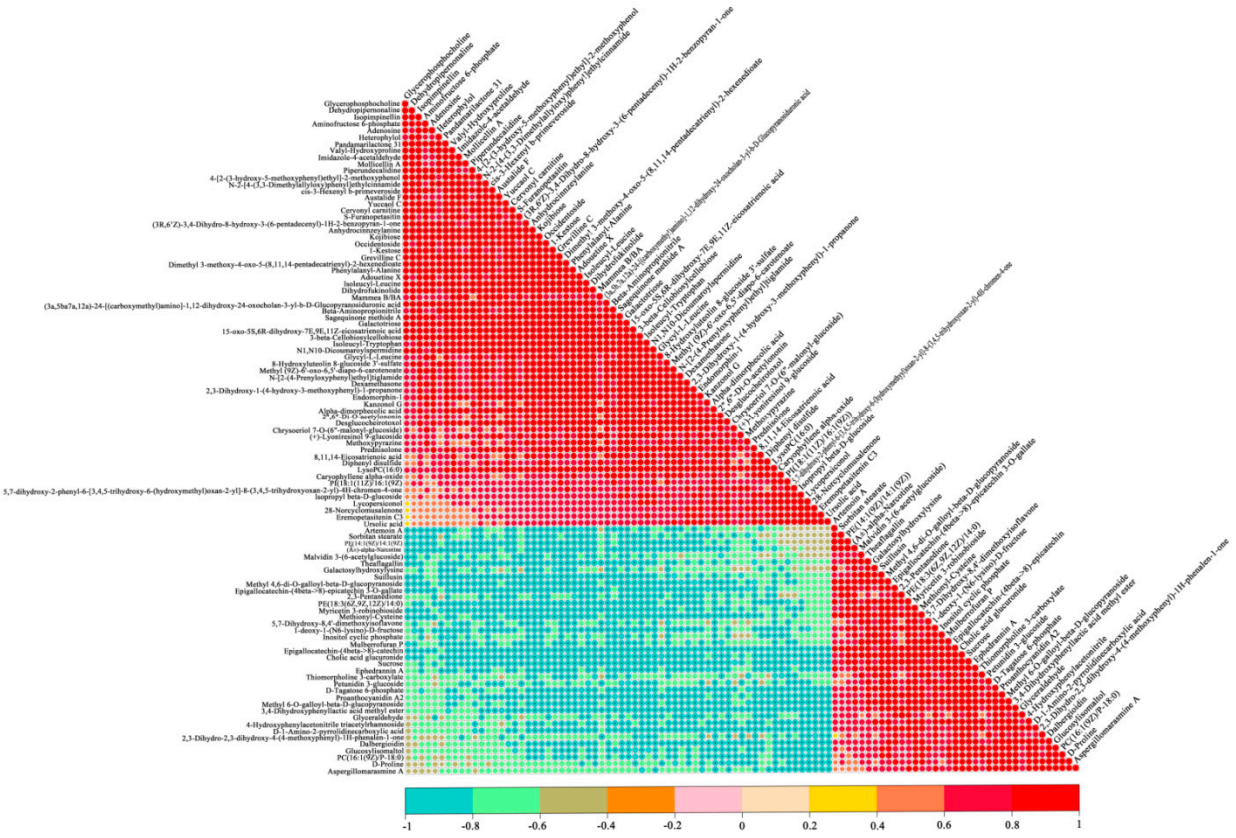


**Figure S7** Correlation maps of metabolites in FGJ during primary fermentation stage

**Table S6** Differential metabolites in FGJ during the three different multi-strain fermentation stages

| NO | Primary fermentation stage (0-8h) | Post fermentation stage (8-16h) | Final fermentation stage (16-24h) |
|---|---|---|---|
| 1 | Dexamethasone | H-LEU-VAL-OH | Phytosphingosine |
| 2 | 2,3-Dihydro-2,3-dihydroxy-4-(4-methoxyphenyl)-1H-phenalen-1-one | Cortisone | Protoanemonin |
| 3 | D-Proline | xi-3-(4-Isopropylphenyl)-2-methylpropanal | 1-Kestose |
| 4 | Beta-Aminopropionitrile | Isoleucyl-Leucine | Tridemorph |
| 5 | Yuccaol C | Dictyoquinazol C | Theaflagallin |
| 6 | 1-Kestose | LysoPE(0:0/14:0) | Rubraflavone C |
| 7 | Theaflagallin | 5,7-Dihydroxy-8,4'-dimethoxyisoflavone | Palmitoylethanolamide |
| 8 | Adenosine | Diospyrin | 5-Decanoyl-2-nonylpyridine |
| 9 | Occidentoside | Palmitoylethanolamide | Methyl 6-O-galloyl-beta-D-glucopyranoside |
| 10 | Petunidin 3-glucoside | Phenylalanyl-Arginine | Pyrophaeophorbide a |
| 11 | Isoleucyl-Leucine | 1-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphate | Tetraacetylethylenediamine |
| 12 | 15-oxo-5S,6R-dihydroxy-7E,9E,11Z-eicosatrienoic acid | Artemoin A | 4,4-Dimethoxy-2-butanone |
| 13 | 1-deoxy-1-(N6-lysino)-D-fructose | PE(20:0/18:1(9Z)) | Bismahanine |
| 14 | 5,7-Dihydroxy-8,4'-dimethoxyisoflavone | Romucosine A | Polyoxyethylene (600) monoricinoleate |
| 15 | Suillusin | Bismahanine | Palmitoleoyl Ethanolamide |
| 16 | Mammea B/BA | PE(P-18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z)) | Isoleucyl-Phenylalanine |
| 17 | Phenylalanyl-Alanine | 3,4-Dihydroxyphenyllactic acid methyl ester | Bisphenol A |
| 18 | Kojibiose | Ursolic acid | 8-Butanoylneosolaniol |

| | | | |
|---|---|---|---|
| 19 | Heterophylol | Dihydrofukinolide | Linamarin |

**Table S6** Differential metabolites in FGJ during the three different multi-strain fermentation stages

| NO | Primary fermentation stage (0-8h) | Post fermentation stage (8-16h) | Final fermentation stage (16-24h) |
|---|---|---|---|
| 20 | Imidazole-4-acetaldehyde | Prenyl caproate | Annocherin A |
| 21 | Aspergillomarasmine A | Aldosterone 18-glucuronide | Methyl 3-(2,3-dihydroxy-3-methylbutyl)-4-hydroxybenzoate |
| 22 | Caryophyllene alpha-oxide | (-)-Epigallocatechin 3-(4-methyl-gallate) | Serylisoleucine |
| 23 | 2'',6''-Di-O-acetylononin | Glycyl-L-Leucine | LysoPC(20:4(5Z,8Z,11Z,14Z)) |
| 24 | Methyl 6-O-galloyl-beta-D-glucopyranoside | Leucyl-Lysine | 6-Methyladenine |
| 25 | Methionyl-Cysteine | Leucyl-Gamma-glutamate | 4-p-Coumaroyl-1,5-quinolactone |
| 26 | Glycerophosphocholine | Dimethyl 3-methoxy-4-oxo-5-(8,11,14-pentadecatrienyl)-2-hexenedioate | D-Galactopyranosyl-(1->3)-D-galactopyranosyl-(1->3)-L-arabinose |
| 27 | N1,N10-Dicoumaroylspermidine | Trifluoromethanesulfonic acid | Lycoperoside D |
| 28 | Artemoin A | Solanocardinol | Macrocarpal I |
| 29 | Kanzonol G | PE(22:4(7Z,10Z,13Z,16Z)/18:1(11Z)) | Pipericine |
| 30 | Grevilline C | Leucyl-Methionine | Malvidin 3-sophoroside 5-glucoside |
| 31 | PI(18:1(11Z)/16:1(9Z)) | Linamarin | Aspartyl-Leucine |
| 32 | cis-3-Hexenyl b-primeveroside | Anhydrocinnzeylanine | (2R*,3R*)-1,2,3-Butanetriol |
| 33 | Myricetin 3-robinobioside | Thiomorpholine 3-carboxylate | 3'-Glucosyl-2',4',6'-trihydroxyacetophenone |
| 34 | Isopropyl beta-D-glucoside | (R) 2,3-Dihydroxy-3-methylvalerate | Edulinine |
| 35 | PC(16:1(9Z)/P-18:0) | Ethoxyquin | PA(18:0/20:4(5Z,8Z,11Z,14Z)) |
| 36 | Galactosylhydroxylysine | 28-Norcyclomusalenone | |
| 37 | Isopimpinellin | Tyrosyl-Serine | |
| 38 | 3,4-Dihydroxyphenyllactic | Lycoperoside D | |

| | | |
|---|---|---|
| | acid methyl ester | |
| 39 | Ursolic acid | Margrapine A |

**Table S6** Differential metabolites in FGJ during the three different multi-strain fermentation stages

| NO | Primary fermentation stage (0-8h) | Post fermentation stage (8-16h) | Final fermentation stage (16-24h) |
|---|---|---|---|
| 39 | Ursolic acid | Margrapine A | |
| 40 | Dihydrofukinolide | Ephedrannin A | |
| 41 | Glyceraldehyde | 1,3-Diphenyl-1-propanone | |
| 42 | 4-Hydroxyphenylacetonitrile triacetylrhamnoside | 3-Methylthiohexyl hexanoate | |
| 43 | Glycyl-L-Leucine | Patuletin 3-(2''-apiosylgentiobioside) | |
| 44 | Alpha-dimorphecolic acid | (3a,5b,7a,12a)-24-[(carboxymethyl)amino]-1,12-dihydroxy-2 4-oxocholan-3-yl-b-D-Glucopyranosiduronic acid | |
| 45 | Valyl-Hydroxyproline | Pipericine | |
| 46 | Methoxypyrazine | N-[2-(4-Prenyloxyphenyl)ethyl]tiglamide | |
| 47 | Malvidin 3-(6-acetylglucoside) | Safflomin C | |
| 48 | Isoleucyl-Tryptophan | L-N-(3-Carboxypropyl)glutamine | |
| 49 | Mollicellin A | (3R, 6'Z)-3,4-Dihydro-8-hydroxy-3-(6-pentadecenyl)-1H-2-benzo pyran-1-one | |
| 50 | Dimethyl 3-methoxy-4-oxo-5-(8,11,14-pentadeca trienyl)-2-hexenedioate | Inositol cyclic phosphate | |
| 51 | Lycopersiconol | Sagequinone methide A | |
| 52 | LysoPC(16:0) | | |
| 53 | Cholic acid glucuronide | | |
| 56 | Eremopetasitenin C3 | | |
| 57 | Austalide F | | |
| 58 | N-2-[4-(3,3-Dimethylallyloxy)phenyl] ethylcinnamide | | |
| 59 | (Â±)-alpha-Narcotine | | |
| 60 | Dalbergioidin | | |

| | |
|---|---|
| 61 | Anhydrocinnzeylanine |

**Table S6** Differential metabolites in FGJ during the three different multi-strain fermentation stages

| NO | Primary fermentation stage (0-8h) | Post fermentation stage (8-16h) | Final fermentation stage (16-24h) |
|---|---|---|---|
| 62 | Thiomorpholine 3-carboxylate | | |
| 63 | Cervonyl carnitine | | |
| 64 | (+)-Lyoniresinol 9-glucoside | | |
| 65 | PE(18:3(6Z,9Z,12Z)/14:0) | | |
| 66 | Methyl 4,6-di-O-galloyl-beta-D-glucopyranoside | | |
| 67 | 2,3-Dihydroxy-1-(4-hydroxy-3-methoxyphenyl)-1-propanone | | |
| 68 | PE(14:1(9Z)/14:1(9Z)) | | |
| 69 | 5,7-dihydroxy-2-phenyl-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-8-(3,4,5-trihydroxyoxan-2-yl)-4H-chromen-4-one | | |
| 70 | D-Tagatose 6-phosphate | | |
| 71 | Sorbitan stearate | | |
| 72 | Aminofructose 6-phosphate | | |
| 73 | 3-beta-Cellobiosylcellobiose | | |
| 74 | 28-Norcyclomusalenone | | |
| 75 | 2,3-Pentanedione | | |
| 76 | Ephedrannin A | | |
| 77 | Sucrose | | |
| 78 | Chrysoeriol 7-O-(6''-malonyl-glucoside) | | |
| 79 | (3a,5b,7a,12a)-24-[(carboxymethyl)amino]-1,12-dihydroxy-24-oxocholan-3-yl-b-D-Glucopyranosiduronic acid | | |
| 93 | Desglucocheirotoxol | | |
| 94 | D-1-Amino-2-pyrrolidinecarboxylic acid | | |

| | | | |
|---|---|---|---|
| 95 | Epigallocatechin-(4beta->8)-epicatechin 3-O-gallate | | |

**Table S6** Differential metabolites in FGJ during the three different multi-strain fermentation stages

| NO | Primary fermentation stage (0-8h) | Post fermentation stage (8-16h) | Final fermentation stage (16-24h) |
|---|---|---|---|
| 96 | Pandamarilactone 31 | | |
| 97 | Sagequinone methide A | | |
| 98 | Methyl (9Z)-6'-oxo-6,5'-diapo-6-carotenoate | | |
| 99 | Diphenyl disulfide | | |
| 100 | 8,11,14-Eicosatrienoic acid | | |
| 101 | Epigallocatechin-(4beta->8)-catechin | | |

**Table S7** Key differential metabolites in FGJ during the three different multi-strain fermentation stages

| Fermentation stages | No | MS2-name | MS2-score | [a]Rt | [b]mz | Mean (0h) | Mean (8h) | Mean (16h) | Mean (24h) | VIP | P-VALUE | Q-VALUE | FOLD-CHANGE |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 1 | 2',6'-Di-O-acetylononin | 0.913 | 77.370 | 515.142 | 0.007 | 0.048 | 0.039 | 0.061 | 1.745 | 0.013 | 0.289 | 7.385 |
| | 2 | 5,7-dihydroxy-2-phenyl-6- | 0.533 | 314.156 | 549.158 | 0.029 | 0.060 | 0.045 | 0.035 | 1.806 | 0.033 | 0.427 | 2.059 |
| | 3 | Ephedrannin A | 0.467 | 46.226 | 557.118 | 0.232 | 0.108 | 0.089 | 0.097 | 2.009 | 0.025 | 0.381 | 0.467 |
| 0-8h | 4 | Proanthocyanidin A2 | 0.432 | 301.176 | 577.132 | 0.013 | 0.006 | 0.006 | 0.005 | 1.967 | 0.003 | 0.172 | 0.469 |
| | 5 | Epigallocatechin-(4beta->8)-catechin | 0.307 | 260.755 | 595.142 | 0.047 | 0.010 | 0.010 | 0.009 | 2.057 | 0 | 0.021 | 0.213 |
| | 6 | 1-Kestose | 0.987 | 63.783 | 527.156 | 0.031 | 0.212 | 0.197 | 0.277 | 1.793 | 0.004 | 0.192 | 6.894 |
| | 7 | 3-beta-Cellobiosylcellobiose | 0.519 | 48.559 | 667.225 | 0.003 | 0.387 | 0.395 | 0.412 | 1.886 | 0.003 | 0.171 | 132.930 |
| | 8 | Galactotriose | 0.377 | 47.635 | 505.175 | 0.050 | 0.443 | 0.404 | 0.461 | 2.056 | 0.0001 | 0.054 | 8.732 |
| | 9 | Linamarin | 0.568 | 69.763 | 248.111 | 0.138 | 0.123 | 0.221 | 0.106 | 1.858 | 0.037 | 1.000 | 0.480 |
| 8-16h | 10 | Dimethyl 3-methoxy-4 | 0.699 | 253.828 | 421.255 | 0.010 | 0.024 | 0.029 | 0.032 | 1.996 | 0.001 | 0.082 | 2.321 |
| | 11 | Palmitoylethanolamide | 0.945 | 623.717 | 300.289 | 0.043 | 0.052 | 0.020 | 0.053 | 1.805 | 0.026 | 1.000 | 0.389 |
| | 12 | Trifluoromethanesulfonic acid | 0.665 | 26.806 | 150.968 | 0.155 | 0.386 | 0.100 | 0.151 | 2.036 | 0.001 | 1.000 | 0.260 |
| 16-24h | 13 | Tetraacetylethylenediamine | 0.899 | 97.560 | 229.117 | 0.150 | 0.074 | 0.099 | 0.202 | 1.861 | 0.029 | 1.000 | 2.029 |

[a] RT, retention time; [b] m/z, mass to charge ratio.

**Part 3: Analyses of VOCs profiles (Figure S8; Table S8-S10)**

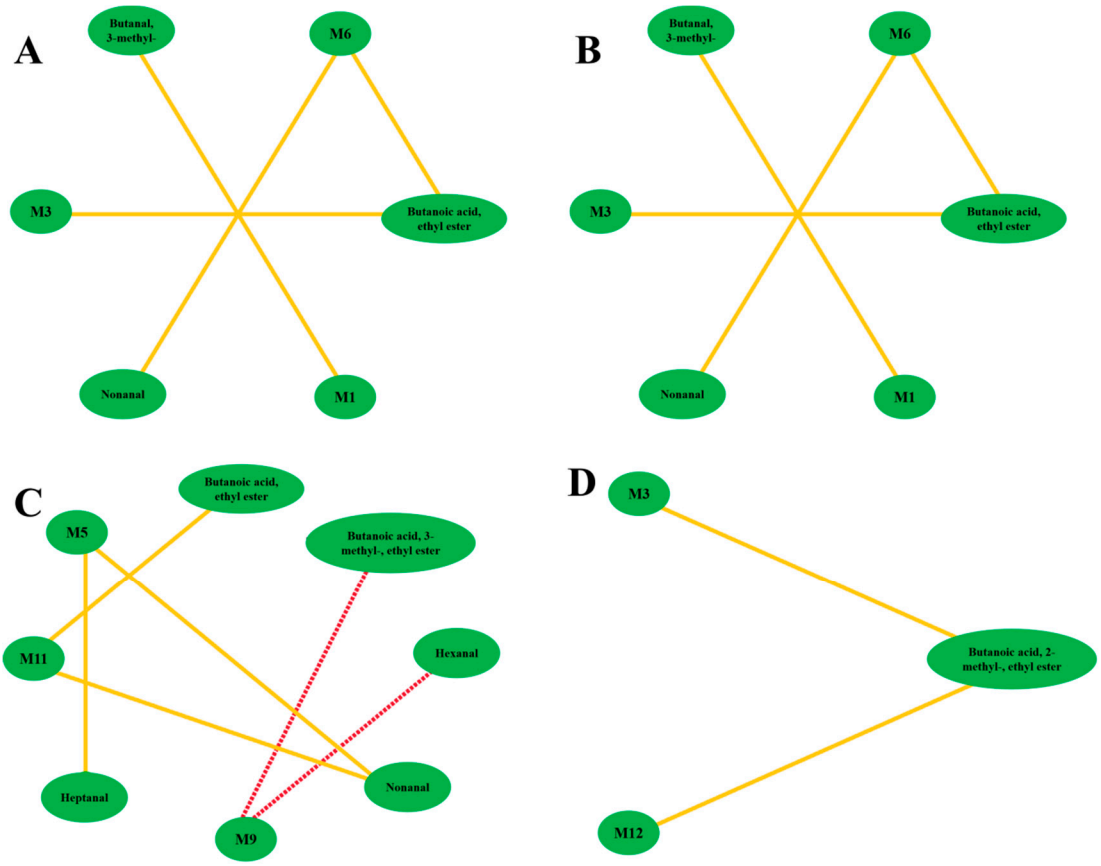


**Figure S8** Networks between the VOCs and saccharides in FGJ based on correlation analyses (A: 0h; B: 8h; C: 16h; D: 24h)

**Table S8** VOCs in FGJ after 24H of multi-strain fermentation

| count | compound | CAS | Formula | mw | Rt |
|---|---|---|---|---|---|
| | **Aldehyde** | | | | |
| 1 | 1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl- | 432-25-7 | $C_{10}H_{16}O$ | 119 | 21.599 |
| 2 | 2-Heptenal, (E)- | 18829-55-5 | $C_7H_{12}O$ | 83 | 13.937 |
| 3 | 2-Hexenal | 505-57-7 | $C_6H_{10}O$ | 62 | 11.084 |
| 4 | 2-Propenal | 107-02-8 | $C_3H_4O$ | 26 | 2.417 |
| 5 | 3-Hexenal | 4440-65-7 | $C_6H_{10}O$ | 69 | 8.494 |
| 6 | 3-Pentenal, 4-methyl- | 5362-50-5 | $C_6H_{10}O$ | 98 | 3.873 |
| 7 | Acetaldehyde | 75-07-0 | $C_2H_4O$ | 42 | 1.732 |
| 8 | Butanal | 123-72-8 | $C_4H_8O$ | 29 | 2.694 |
| 9 | Butanal, 3-methyl- | 590-86-3 | $C_5H_{10}O$ | 71 | 3.193 |
| 10 | Heptanal | 111-71-7 | $C_7H_{14}O$ | 70 | 9.868 |
| 11 | Hexanal | 66-25-1 | $C_6H_{12}O$ | 56 | 6.899 |
| 12 | Methional | 3268-49-3 | $C_4H_8OS$ | 48 | 17.459 |
| 13 | Nonanal | 124-19-6 | $C_9H_{18}O$ | 98 | 15.915 |
| 14 | Octanal | 124-13-0 | $C_8H_{16}O$ | 84 | 12.971 |
| 15 | Pentanal | 110-62-3 | $C_5H_{10}O$ | 58 | 4.296 |
| 16 | Propanal, 2-methyl- | 78-84-2 | $C_4H_8O$ | 72 | 2.189 |
| | **Ester** | | | | |
| 17 | 2-Hexen-1-ol, acetate, (Z)- | 56922-75-9 | $C_8H_{14}O_2$ | 88 | 14.319 |
| 18 | 2-Propenoic acid, 2-methyl-, ethenyl ester | 4245-37-8 | $C_6H_8O_2$ | 41 | 8.226 |
| 19 | 2,4-Decadienoic acid, ethyl ester, (E,Z)- | 3025-30-7 | $C_{12}H_{20}O_2$ | 81 | 26.645 |
| 20 | 2(3H)-Furanone, 5-butyldihydro- | 104-50-7 | $C_8H_{14}O_2$ | 85 | 28.062 |
| 21 | 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)- | 17092-92-1 | $C_{11}H_{16}O_2$ | 111 | 35.999 |
| 22 | 3-Hexen-1-ol, acetate, (Z)- | 3681-71-8 | $C_8H_{14}O_2$ | 67 | 13.839 |
| 23 | Acetic acid ethenyl ester | 108-05-4 | $C_4H_6O_2$ | 86 | 4.284 |
| 24 | Acetic acid, hexyl ester | 142-92-7 | $C_8H_{16}O_2$ | 56 | 12.572 |
| 25 | Acetic acid, methoxy-, ethyl ester | 3938-96-3 | $C_5H_{10}O_3$ | 61 | 2.821 |
| 26 | Acetic acid, methyl ester | 79-20-9 | $C_3H_6O_2$ | 74 | 2.296 |

**Table S8** VOCs in FGJ after 24H of multi-strain fermentation

| count | compound | CAS | Formula | mw | Rt |
|---|---|---|---|---|---|
| 27 | Butanoic acid, 2-methyl-, ethyl ester | 7452-79-1 | $C_7H_{14}O_2$ | 102 | 6.185 |
| 28 | Butanoic acid, 3-hydroxy-, ethyl ester | 5405-41-4 | $C_6H_{12}O_3$ | 195 | 19.254 |
| 29 | Butanoic acid, 3-methyl-, ethyl ester | 108-64-5 | $C_7H_{14}O_2$ | 88 | 6.609 |
| 30 | Butanoic acid, ethyl ester | 105-54-4 | $C_6H_{12}O_2$ | 71 | 5.744 |
| 31 | Butyrolactone | 96-48-0 | $C_4H_6O_2$ | 42 | 21.656 |
| 32 | Carbamic acid, methylnitroso-, ethyl ester | 615-53-2 | $C_4H_8N_2O_3$ | 30 | 1.567 |
| 33 | Diethyl carbonate | 105-58-8 | $C_5H_{10}O_3$ | 91 | 7.61 |
| 34 | Ethyl tiglate | 5837-78-5 | $C_7H_{12}O_2$ | 83 | 11.473 |
| 35 | Formic acid, ethenyl ester | 692-45-5 | $C_3H_4O_2$ | 29 | 2.409 |
| 36 | Hexanoic acid, 3-hydroxy-, ethyl ester | 2305-25-1 | $C_8H_{16}O_3$ | 46 | 23.113 |
| 37 | Hexanoic acid, 5-oxo-, ethyl ester | 13984-57-1 | $C_8H_{14}O_3$ | 108 | 24.115 |
| 38 | Hexanoic acid, ethyl ester | 123-66-0 | $C_8H_{16}O_2$ | 88 | 11.420 |
| 39 | Isobutyl acetate | 110-19-0 | $C_6H_{12}O_2$ | 43 | 6.704 |
| 40 | Pentanoic acid, ethyl ester | 539-82-2 | $C_7H_{14}O_2$ | 88 | 8.409 |
| 41 | Propanoic acid, 2-oxo-, ethyl ester | 617-35-6 | $C_5H_8O_3$ | 43 | 12.455 |
| 42 | Propanoic acid, ethyl ester | 105-37-3 | $C_5H_{10}O_2$ | 57 | 3.901 |
| | **Ketone** | | | | |
| 43 | 1-Penten-3-one | 1629-58-9 | $C_5H_8O$ | 55 | 5.257 |
| 44 | 1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl- | 20189-42-8 | $C_7H_9NO_2$ | 67 | 34.802 |
| 45 | 2-Heptanone, 6-methyl- | 928-68-7 | $C_8H_{16}O$ | 71 | 21.181 |
| 46 | 2-Octanone | 111-13-7 | $C_8H_{16}O$ | 58 | 12.893 |
| 47 | 2-Pentadecanone, 6,10,14-trimethyl- | 502-69-2 | $C_{18}H_{36}O$ | 137 | 32.296 |
| 48 | 2,3-Hexanedione | 3848-24-6 | $C_6H_{10}O_2$ | 43 | 8.312 |
| 50 | 2(5H)-Furanone | 497-23-4 | $C_4H_4O_2$ | 84 | 24.528 |
| 51 | 3-Chloro-2,4-pentanedione | 1694-29-7 | $C_5H_7ClO_2$ | 119 | 12.546 |
| 52 | 3-Hexanone, 4-methyl- | 17042-16-9 | $C_7H_{14}O$ | 85 | 19.708 |
| 53 | 5-Hepten-2-one, 6-methyl- | 110-93-0 | $C_8H_{14}O$ | 111 | 14.384 |
| 54 | Acetoin | 513-86-0 | $C_4H_8O_2$ | 45 | 12.917 |

**Table S8** VOCs in FGJ after 24H of multi-strain fermentation

| count | compound | CAS | Formula | mw | Rt |
|---|---|---|---|---|---|
| 55 | Acetone | 67-64-1 | $C_3H_6O$ | 58 | 2.207 |
| 56 | Cyclononanone | 3350-30-9 | $C_9H_{16}O$ | 55 | 19.569 |
| | **Acid** | | | | |
| 57 | Acetic acid | 64-19-7 | $C_2H_4O_2$ | 60 | 17.418 |
| | **Alcohol** | | | | |
| 58 | 1-Butanol | 71-36-3 | $C_4H_{10}O$ | 56 | 9.176 |
| 59 | 1-Heptanol, 4-methyl- | 817-91-4 | $C_8H_{18}O$ | 41 | 20.456 |
| 60 | 1-Hexen-3-ol | 4798-44-1 | $C_6H_{12}O$ | 57 | 12.161 |
| 61 | 1-Nonanol | 143-08-8 | $C_9H_{20}O$ | 56 | 22.882 |
| 62 | 1-Octen-3-ol | 3391-86-4 | $C_8H_{16}O$ | 72 | 17.615 |
| 63 | 1-Penten-3-ol | 616-25-1 | $C_5H_{10}O$ | 57 | 9.557 |
| 64 | 2-Chloroethanol | 107-07-3 | $C_2H_5ClO$ | 44 | 3.519 |
| 65 | 2-Hexen-1-ol, (E)- | 928-95-0 | $C_6H_{12}O$ | 67 | 16.494 |
| 66 | 3-Buten-1-ol, 3-methyl- | 763-32-6 | $C_5H_{10}O$ | 67 | 12.053 |
| 67 | 3-Hexen-1-ol, (E)- | 928-97-2 | $C_6H_{12}O$ | 74 | 15.881 |
| 68 | 4-Methyl-2-hexanol | 2313-61-3 | $C_7H_{16}O$ | 71 | 14.157 |
| 69 | Ethanol | 64-17-5 | $C_2H_6O$ | 46 | 3.550 |
| 70 | Methyl Alcohol | 67-56-1 | $CH_4O$ | 31 | 2.961 |
| | **Other** | | | | |
| 71 | 1-Penten-3-one, 2-methyl- | 25044-01-3 | $C_6H_{10}O$ | 69 | 6.474 |
| 72 | 1,4-Oxathiane | 15980-15-1 | $C_4H_8OS$ | 104 | 15.021 |
| 73 | 2-Cyclohexen-1-ol, 2,6,6-trimethyl- | 54345-59-4 | $C_9H_{16}O$ | 125 | 31.210 |
| 74 | 2,5-Furandione, 3,4-dimethyl- | 766-39-2 | $C_6H_6O_3$ | 54 | 24.022 |
| 75 | Acetamide | 60-35-5 | $C_2H_5NO$ | 59 | 24.910 |
| 76 | Acetic anhydride | 108-24-7 | $C_4H_6O_3$ | 43 | 2.821 |
| 77 | Cyclobutane, methylene- | 1120-56-5 | $C_5H_8$ | 52 | 1.628 |
| 78 | Dodecane | 112-40-3 | $C_{12}H_{26}$ | 85 | 10.238 |
| 79 | Hexanenitrile | 628-73-9 | $C_6H_{11}N$ | 54 | 13.188 |

**Table S8** VOCs in FGJ after 24H of multi-strain fermentation

| count | compound | CAS | Formula | mw | Rt |
|---|---|---|---|---|---|
| 80 | Isopropylcyclobutane | 872-56-0 | $C_7H_{14}$ | 55 | 2.448 |
| 81 | Pinocarvone | 30460-92-5 | $C_{10}H_{14}O$ | 108 | 20.320 |
| 82 | Pyrazine, tetramethyl- | 1124-11-4 | $C_8H_{12}N_2$ | 136 | 18.169 |
| 83 | Pyrazine, trimethyl- | 14667-55-1 | $C_7H_{10}N_2$ | 122 | 16.291 |
| 84 | Succinimide | 123-56-8 | $C_4H_5NO_2$ | 99 | 38.172 |
| 85 | Tridecane | 629-50-5 | $C_{13}H_{28}$ | 57 | 13.337 |

**Table S9** Carbohydrates (mean relative abundance > 0.5%) in FGJ during multi-strain fermentation stages

| No | Metabolites | [a]RT(min) | [b]m/z | Mean (0h) | Mean (8h) | Mean (16h) | Mean (24h) | Class |
|---|---|---|---|---|---|---|---|---|
| M1 | L-Gulose | 67.158 | 203.051 | 15.296 | 6.805 | 14.354 | 18.427 | Carbohydrates and carbohydrate conjugates |
| M2 | Phenylethyl primeveroside | 281.914 | 439.155 | 0.847 | 0.866 | 0.836 | 0.608 | Carbohydrates and carbohydrate conjugates |
| M3 | 2-O-Acetylarbutin | 217.317 | 315.104 | 1.395 | 1.404 | 1.367 | 1.300 | Carbohydrates and carbohydrate conjugates |
| M4 | Hydroxytyrosol | 249.069 | 317.119 | 11.169 | 11.130 | 10.886 | 11.002 | Amino acids, peptides, and analogues |
| M5 | 1-O-glucoside | 291.569 | 477.192 | 1.161 | 1.179 | 1.163 | 1.181 | Carbohydrates and carbohydrate conjugates |
| M6 | Kanokoside A | 277.363 | 393.115 | 0.619 | 0.608 | 0.603 | 0.609 | Carbohydrates and carbohydrate conjugates |
| M7 | Garcimangosone D | 293.056 | 343.172 | 1.523 | 1.305 | 1.711 | 0.902 | Carbohydrates and carbohydrate conjugates |
| M8 | Jasmolone glucoside | 214.414 | 180.086 | 7.531 | 7.397 | 7.793 | 7.684 | Carbohydrates and carbohydrate conjugates |
| M9 | Glucosamine | 458.434 | 180.086 | 1.501 | 1.407 | 1.411 | 1.501 | Carbohydrates and carbohydrate conjugates |
| M10 | L-Galactose | 136.806 | 198.096 | 44.125 | 48.468 | 51.924 | 48.579 | Carbohydrates and carbohydrate conjugates |
| M11 | Glucosylisomaltol | 47.381 | 289.091 | 0.717 | 0.644 | 0.586 | 0.593 | Carbohydrates and carbohydrate conjugates |
| M12 | Ethyleta-D-glucopyranoside | 101.955 | 209.101 | 4.434 | 4.350 | 4.291 | 4.312 | Carbohydrates and carbohydrate conjugates |

[a] RT, retention time; [b]m/z, mass to charge ratio.

**Table S10** Carboxylic acids and derivatives, and fatty acyls (mean relative abundance > 0.5%) in FGJ during multi-strain fermentation stages

| No | Metabolites | [a]RT(min) | [b]m/z | Mean (0h) | Mean (8h) | Mean (16h) | Mean (24h) | Class |
|---|---|---|---|---|---|---|---|---|
| M1 | Diethyl fumarate | 187.770 | 173.078 | 4.698 | 4.675 | 4.388 | 4.818 | Fatty Acyls |
| M2 | Betaine | 781.100 | 118.086 | 5.702 | 5.919 | 5.883 | 5.904 | Carboxylic acids and derivatives |
| M3 | Bisnorbiotin | 71.540 | 217.067 | 5.334 | 6.158 | 5.798 | 5.456 | Organic acids and derivatives |
| M4 | D-Proline | 47.620 | 116.070 | 36.555 | 34.105 | 34.187 | 33.175 | Carboxylic acids and derivatives |
| M5 | Kanokoside A | 291.560 | 477.192 | 1.161 | 1.179 | 1.163 | 1.181 | Carboxylic acids and derivatives |
| M6 | 3,3,5-triiodo-L-thyronine- | 88.160 | 132.101 | 21.848 | 22.095 | 21.062 | 22.312 | Carboxylic acids and derivatives |
| M7 | 6-Aminopenicillanic acid | 86.730 | 217.067 | 1.377 | 1.379 | 1.346 | 1.412 | Carboxylic acids and derivatives |
| M8 | L-Histidine | 42.330 | 156.076 | 2.704 | 2.681 | 2.557 | 2.660 | Carboxylic acids and derivatives |
| M9 | 1-deoxy-1-(N6-lysino)-D- | 39.680 | 134.044 | 1.875 | 1.396 | 1.299 | 1.218 | Carboxylic acids and derivatives |
| M10 | Lauroyl diethanolamide | 494.630 | 288.252 | 5.971 | 6.020 | 6.070 | 6.290 | Fatty Acyls |
| M11 | (alpha-D-mannosyl)7-beta- | 43.620 | 90.055 | 7.669 | 7.122 | 7.177 | 6.980 | Carboxylic acids and derivatives |
| M12 | 2-Methyl-3-hydroxyvaleric | 249.040 | 133.086 | 1.574 | 1.559 | 1.506 | 1.488 | Fatty Acyls |
| M13 | L-Glutamic acid | 40.560 | 148.060 | 5.577 | 4.297 | 3.644 | 3.520 | Carboxylic acids and derivatives |
| M14 | Kojibiose | 46.980 | 325.112 | 7.882 | 9.383 | 9.324 | 8.996 | Fatty Acyls |
| M15 | N-Acryloylglycine | 69.110 | 130.050 | 2.056 | 1.962 | 2.225 | 1.965 | Carboxylic acids and derivatives |
| M16 | L-Allothreonine | 43.780 | 120.065 | 4.112 | 3.884 | 3.924 | 3.917 | Organic acids and derivatives |
| M17 | L-Methionine | 55.430 | 150.058 | 2.624 | 2.744 | 2.670 | 2.719 | Organic acids and derivatives |
| M18 | N2-Fructopyranosylarginine | 44.230 | 337.170 | 1.286 | 1.524 | 1.646 | 1.563 | Carboxylic acids and derivatives |
| M19 | (2E,4E)-2,7-Dimethyl-2,4-o | 165.380 | 199.100 | 1.535 | 1.494 | 1.743 | 1.420 | Fatty Acyls |
| M20 | Argininosuccinic acid | 48.780 | 291.129 | 5.165 | 5.072 | 4.673 | 4.907 | Carboxylic acids and derivatives |
| M21 | Dihydroceramide | 663.810 | 330.299 | 1.506 | 1.514 | 1.493 | 1.552 | Carboxylic acids and derivatives |
| M22 | Vinylacetylglycine | 793.910 | 144.065 | 3.097 | 3.551 | 3.031 | 3.27 | Carboxylic acids and derivatives |
| M23 | Docosanamide | 674.180 | 340.356 | 4.009 | 2.092 | 5.347 | 4.619 | Fatty Acyls |
| M24 | Histidinyl-Asparagine | 44.270 | 270.117 | 1.823 | 1.759 | 1.760 | 1.791 | Carboxylic acids and derivatives |
| M25 | Corchoionol C 9-glucoside | 485.150 | 387.191 | 1.323 | 1.260 | 1.245 | 1.208 | Fatty Acyls |
| M26 | Palmitic acid | 477.190 | 274.273 | 50.276 | 44.012 | 48.891 | 48.097 | Fatty Acyls |
| M27 | 2,4,12-Octadecatrienoic | 675.110 | 334.310 | 2.582 | 2.333 | 2.365 | 2.572 | Fatty Acyls |

[a] RT, retention time; [b]m/z, mass to charge ratio.