**Supplementary data**

**Fig. S1.** PCA score plots derived from non-targeted metabolite profiling of 11 *meju* types analyzed using GC–TOF-MS (A) and UHPLC–Orbitrap-MS/MS (B). PCA Score plots for *meju* samples: (■); M1 (■), M2 (■), M3 (■), M4 (■), M5 (■), M6 (■), M7 (■), M8 (■), M9 (■), M10 (■), M11 (■).
Table S1. Tentatively identified meju metabolites from different materials based on the GC-TOF-MS analysis.

| S.No. | Tentative identifications* | RT** (min) | Identified ion (m/z) | Mass Fragment pattern (m/z)*** | TMS** |
|-------|---------------------------|------------|----------------------|--------------------------------|-------|
| **Amino acids** | | | | | |
| 1 | Valine | 6.7 | 144 | 73 144 147 218 100 59 75 145 74 | 2 |
| 2 | Leucine | 7.2 | 158 | 158 73 102 159 100 59 75 74 | 2 |
| 3 | Glycine | 7.6 | 174 | 73 174 86 147 59 100 175 133 | 3 |
| 4 | Serine | 8.1 | 204 | 73 204 218 100 147 75 74 | 3 |
| 5 | Threonine | 8.3 | 57 | 73 57 117 101 219 218 147 | 3 |
| 6 | Aspartic Acid | 9.5 | 232 | 73 232 100 147 75 74 117 233 | 3 |
| 7 | Phenylalanine | 10.4 | 218 | 73 218 192 100 147 75 74 219 | 2 |
| 8 | Ornithine | 11.8 | 142 | 73 142 174 59 86 74 147 100 143 | 4 |
| 9 | Lysine | 12.5 | 156 | 73 156 174 59 86 128 100 74 | 4 |
| 10 | Histidine | 12.5 | 154 | 73 203 154 147 75 74 103 59 | 3 |
| 11 | Tyrosine | 12.6 | 100 | 73 218 100 147 75 219 74 103 | 3 |
| 12 | Tryptophan | 14.4 | 202 | 73 202 75 203 74 55 204 117 129 | 3 |
| **Fatty acids** | | | | | |
| 13 | Butanoic Acid | 8.7 | 75 | 73 147 75 101 189 117 74 133 59 | 3 |
| 14 | Hexadecanoic Acid | 13.2 | 132 | 117 75 73 132 129 55 145 131 | 1 |
| 15 | Oleic Acid | 14.2 | 98 | 75 117 73 55 129 145 81 96 67 84 | 1 |
| 16 | Linolenic Acid | 14.3 | 335 | 73 79 73 55 67 95 117 129 81 93 | 1 |
| **Sugar & sugar derivatives** | | | | | |
| 17 | Glycerol | 7.3 | 117 | 73 117 103 205 147 218 133 | 3 |
| 18 | Pinitol | 11.9 | 133 | 73 147 133 217 260 86 191 103 74 75 | 5 |
| 19 | Adonitol | 12.1 | 103 | 73 103 147 217 68 67 149 89 74 129 | 5 |
| 20 | Glucosamine | 13.6 | 202 | 73 147 129 87 75 117 202 74 | 4 |
| 21 | Sucrose | 16.7 | 361 | 73 147 103 217 361 129 169 | 7 |
| 22 | Maltose | 16.8 | 204 | 73 204 147 103 129 217 75 74 | 8 |
| **Etc** | | | | | |
| 23 | Urea | 6.9 | 189 | 147 73 189 171 66 148 74 99 59 | 2 |
| 24 | Benzoic Acid | 7.0 | 105 | 105 77 179 165 51 180 50 | 1 |
| **Non-Identifications** | | | | | |
| 25 | N.I. I | 9.4 | 103 | 147 103 117 133 59 129 11 148 | 4 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 26 | N.I. 2 | 9.9 | 129 | 73 129 147 75 85 157 247 133 | 3 |
| 27 | N.I. 3 | 14.2 | 262 | 75 73 55 67 81 129 79 95 117 | 1 |
| 28 | N.I. 4 | 15.3 | 331 | 73 75 55 67 81 129 131 117 | 2 |
| 29 | N.I. 5 | 17.2 | 361 | 73 191 147 361 103 129 217 | 7 |

*Tentative metabolites based on VIP>1.0 and \( p<0.05 \) based on PLS-DA and one-way ANOVA analysis, respectively.

**RT, and TMS indicates retention time, and trimethylsilyl, respectively.
# Table S2. Tentatively identified meju metabolites from different materials based on the UHPLC-Orbitrap-MS/MS analysis.

| S. No. | Tentative identifications* | RT** (min) | [M-H]^- | [M+H]^+ | MW ** | Elemental composition [M+H]^+ | Error (ppm) | MS^n fragment pattern (m/z) | ID ** |
|--------|-----------------------------|------------|---------|---------|-------|-------------------------------|-------------|--------------------------------|------|
| **Isoflavonoids** | | | | | | | | | |
| 30 | Daidzin | 4.51 | 415.1034 | 417.1169 | 416 | C21H21O9 | -2.778 | 417>287,269,255>254,227,211 | Ref [1, 2] |
| 31 | Glycitin | 4.61 | 445.1140 | 447.1277 | 446 | C22H23O10 | -1.841 | 447>429,316,285>270,229 | Ref [1, 2] |
| 32 | Genistin | 4.95 | 431.0980 | 433.1116 | 432 | C21H21O10 | -3.055 | 433>415,313,271>253,243,215,152 | Ref [1, 2] |
| 33 | Malonyldaidzin | 4.95 | 501.1977 | 503.1169 | 502 | C24H23O12 | -1.933 | | |
| 34 | Malonylglycitin | 5.40 | 531.1149 | 533.1276 | 532 | C25H25O13 | -1.383 | 531>487,431,269>268,224,180 | Ref [2] |
| 35 | Malonylgenistin | 5.33 | 517.1232 | 519.1120 | 518 | C24H23O13 | -2.537 | 519>433,271>270,242,148,148 | Ref [2] |
| 36 | Acetyldaidzin | 5.21 | 457.1138 | 459.1274 | 458 | C23H23O10 | -2.599 | | |
| 37 | Acetylglycitin | 5.30 | 487.1777 | 489.1380 | 488 | C24H25O11 | -2.265 | | |
| 38 | Acetylgenistin | 5.71 | 473.1079 | 475.1223 | 474 | C23H23O11 | -2.416 | 475>457,379,313,>242,215,152 | Ref [2] |
| 39 | Glycitein | 5.87 | 283.0615 | 285.0750 | 284 | C16H13O5 | -2.491 | 285>283,267,251,215 | Ref [1, 2] |
| 40 | Hydroxyglycitein | 6.29 | 301.0701 | 299.0563 | 300 | C16H13O6 | -1.975 | | |
| 41 | Hydroxygentistein | 5.77 | 285.0405 | 283.0615 | 284 | C15H11O6 | -2.838 | 285>283,261,215 | Ref [1, 2] |
| **Soyasaponin** | | | | | | | | | |
| 42 | Soyasaponin A2 | 5.43 | 1105.5431 | 1107.5563 | 1106 | C53H87O24 | -2.826 | 1107>945,959,421>239,227,184 | HMDB | |
| 44 | Soyasaponin Bf | 6.47 | 925.4783 | 927.4949 | 926 | C47H75O18 | -1.554 | 925>923,717,>567,511,471 | Ref [3] |
| 45 | Soyasaponin Aa | 6.44 | 1363.6152 | 1365.6313 | 1364 | C64H99O31 | -1.723 | | |
| 46 | Soyasaponin Ab | 6.54 | 1435.6367 | 1437.6517 | 1466 | C67H105O33 | -1.828 | | |
| 47 | Soyasaponin Ac | 6.68 | 1201.5640 | 1203.5775 | 1202 | C58H91O26 | -1.495 | 1201>1159,967,719,605,473 | Ref [4] |
| 48 | Soyasaponin Ag | 6.75 | 1171.5514 | 1173.5680 | 1172 | C57H89O25 | -0.643 | 1171>1129,833,719,605>473 | Ref [4] |
| 49 | Soyasaponin Af | 6.79 | 1273.5848 | 1275.6003 | 1274 | C61H95O28 | -0.077 | 1273>1231,1043,749,605>473 | Ref [4] |
| 50 | Soyasaponin Ah | 6.82 | 1243.5732 | 1245.5870 | 1244 | C60H93O27 | 2.440 | 1243>1231,1043,749,605 | Ref [4] |
| 51 | Soyasaponin I | 7.05 | 941.5108 | 943.5252 | 942 | C48H79O18 | -1.280 | 943>325,797,599>581,423,351 | Ref [2, 5] |
| 52 | Soyasaponin II | 7.26 | 911.4996 | 913.5142 | 912 | C47H77O17 | -3.171 | 911>893,765,457>437,371 | Ref [2, 5] |
| 53 | Soyasaponin III | 7.29 | 795.4519 | 797.4665 | 796 | C42H69O13 | -1.874 | 797>779,599,423,365>203 | Ref [2, 5] |
| 54 | Soyasaponin IV | 7.39 | 765.4418 | 767.4562 | 766 | C41H67O13 | -1.874 | 765>721,615,457 | Ref [2, 5] |
| **Glycerophospholipids** | | | | | | | | | |
| 55 | LysoPC18:3 | 8.12 | 562.3145 | 518.3217 | 517 | C26H49NO7P | -4.622 | 518>500,258,184>162 | Ref [5] |
| 56 | LysoPC18:2 | 8.51 | 518.2885 | 520.3381 | 519 | C26H51NO7P | -3.490 | 520>502,443,397,337>323 | Ref [5] |
| 57 | LysoPC16:0 | 8.81 | 540.3309 | 496.3376 | 497 | C24H51NO7P | -4.323 | 496>478,466,421>419,103 | Ref [5] |
| Compound                              | RT   | MW       | ID         | Ref               |
|--------------------------------------|------|----------|------------|-------------------|
| **LysoPC18:1**                       | 9.04 | 566.3459 | 522.3529   | 521 C26H53NO7P    | 4.797 522>504,445>419,309 Ref [5] |
| **LysoPC18:0**                       | 9.73 | 568.3617 | 524.3691   | 523 C26H55NO7P    | 3.787 524>506,447,341>311 Ref [5] |

**Flavonoids**

| Compound                              | RT   | MW       | ID         | Ref               |
|--------------------------------------|------|----------|------------|-------------------|
| Naringenin-7-O-glucoside             | 3.89 | 433.1143 | 435.117    | 434 C21H23O10     | -1.547 433>415,271,205>150 Ref [6] |
| Naringenin                           | 6.38 | 271.0611 | 273.0645   | 272 (-) C15H11O5  | -0.246 |
| Luteolin 7-rutinoside                | 4.64 | 609.1449 | 611.1585   | 610 (-) C27H29O16 | -1.983 609>591,429,285,255,179 Ref [4] |
| Luteolin 7-methyl ether              | 5.23 | 299.0561 | 301.0699   | 300 C16H13O6      | -2.274 299>284,253>227,184 Ref [4] |
| Luteolin                             | 5.49 | 285.0406 | 287.0542   | 286 C15H11O6      | -2.733 285>256,241>213 Ref [4] |

**Oxylipins**

| Compound                              | RT   | MW       | ID         | Ref               |
|--------------------------------------|------|----------|------------|-------------------|
| 9,12,13-TriHOME                      | 6.54 | 329.2329 | 331.1872   | 330 (-) C18H33O5  | -1.420 329>311,293>185,171 Ref [7] |
| 9,10-DiHODE                          | 7.12 | 311.2223 | 313.2362   | 312 (-) C18H31O4  | -1.583 311>293,275,255,157 Ref [7] |
| 9(S)-HpODE                            | 7.66 | 311.2225 | 313.2368   | 312 (-) C18H33O4  | -3.712 311>293,281>275,249,191,139 Ref [7] |
| 12,13-DiHOME                         | 8.12 | 313.2375 | 315.2516   | 314 (-) C18H33O4  | -2.818 313>295,277>195,183 Ref [7] |
| 13-HODE                              | 8.96 | 295.2275 | 297.2613   | 296 (-) C18H31O3  | -1.111 295>277>275,259,233 Ref [7] |
| 9-OxoODE                             | 9.20 | 293.2124 | 295.2257   | 294 (-) C18H29O3  | 0.416 293>275,265>257,255 HMDB |

**Non-identification**

| Compound | RT   | MW       | ID         | Ref               |
|----------|------|----------|------------|-------------------|
| N.I. 6   | 5.97 | 1089.5463| 1091.5616  | 1090 - 1091>929,731,581,423,365>203 - |
| N.I. 7   | 6.04 | 1073.5524| 1075.5670  | 1074 - 1073>1055,747,589>367 - |
| N.I. 8   | 8.29 | 416.2909 | 418.3046   | 417 - 418>400,372>355,243 - |
| N.I. 9   | 9.14 | 426.2683 | 428.2812   | 427 - 428>410,364>318,263 - |
| N.I. 10  | 9.37 | 408.2761 | 410.2885   | 409 - 410>392,263>129 - |
| N.I. 11  | 9.50 | 438.3329 | 440.3465   | 439 - 438>421,395>377,351,131 - |
| N.I. 12  | 9.67 | 380.2808 | 382.2939   | 381 - 382>264,336>318,263 - |
| N.I. 13  | 10.50| 378.3006 | 380.3141   | 379 - 380>362,334,263>261,184 - |

*Tentative metabolites based on VIP>1.0 and \( p<0.05 \) based on PLS-DA and one-way ANOVA analysis, respectively.

**RT, MW, ID, Ref, and HMDB indicates retention time, molecular weight, identification, reference, and https://hmdb.ca/, respectively.

***Superscript 'a' indicates the \([M-FA+H]\).
Supplementary references

1. Lee S, Seo M-H, Oh D-K, Lee CH. 2014. Targeted metabolomics for Aspergillus oryzae-mediated biotransformation of soybean isoflavones, showing variations in primary metabolites. *Biosci. Biotech. Bioch.* **78**: 167-174.

2. Lee SY, Lee S, Lee S, Oh JY, Jeon EJ, Ryu HS, *et al.* 2014. Primary and secondary metabolite profiling of doenjang, a fermented soybean paste during industrial processing. *Food Chem.* **165**: 157-166.

3. Lee S-Y, Kim J-S, Shim S-H, Kang S-S. 2011. Soyasaponins from Soybean Flour Medium for the Liquid Culture of Ganoderma applanatum. *B Korean Chem Soc.* **32**: 3650-3654.

4. Suh DH, Jung ES, Park HM, Kim SH, Lee S, Jo YH, *et al.* 2016. Comparison of metabolites variation and antiobesity effects of fermented versus nonfermented mixtures of Cudrania tricuspidata, Lonicera caerulea, and soybean according to fermentation in vitro and in vivo. *PLoS One.* **11**.

5. Kwon YS, Lee S, Lee SH, Kim HJ, Lee CH. 2019. Comparative Evaluation of Six Traditional Fermented Soybean Products in East Asia: A Metabolomics Approach. *Metabolites.* **9**: 183.

6. Zeng X, Su W, Zheng Y, Liu H, Li P, Zhang W, *et al.* 2018. UFLC-Q-TOF-MS/MS-based screening and identification of flavonoids and derived metabolites in human urine after oral administration of Exocarpium Citri Grandis extract. *Molecules.* **23**: 895.

7. Strassburg K, Huijbrechts AM, Kortekaas KA, Lindeman JH, Pedersen TL, Dane A, *et al.* 2012. Quantitative profiling of oxylipins through comprehensive LC-MS/MS analysis: application in cardiac surgery. *Anal Bional Chem.* **404**: 1413-1426.