# Supplementary Materials: Metabolomics Reveals Quality Characterization of Commercial Gochujang (Fermented Pepper Paste)

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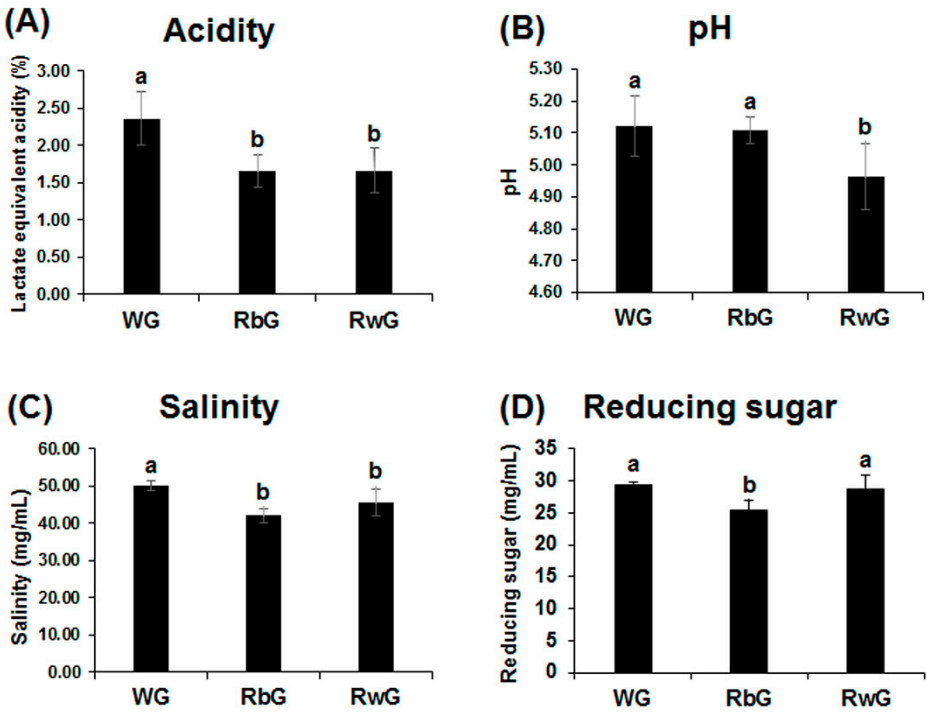


**Figure S1.** Graphs of the results for acidity (**A**), pH (**B**), salinity (**C**), and reducing sugar content (**D**) for physicochemical characteristics of commercial gochujang samples according to the different cereal grains used. All assays were conducted in duplicate, and values are the average of each group of gochujang (WG, wheat gochujang; RbG, brown rice gochujang; RwG, white rice gochujang). Different letters over the bars indicate that values were statistically significant by analysis of variance (ANOVA) followed by Duncan's multiple-range test ($p$-value < 0.05).

**Table S1.** List of significantly different metabolites according to type of cereal grains used in commercial gochujang based on GC-TOF-MS data.

| No. | Tentative Metabolites [a] | VIP 1 [a] | VIP 2 [a] | $t_R$ [b] (min) | MS Fragment Ion (*m*/*z*) | Identified Ion [c] (*m*/*z*) | TMS [d] | ID [e] |
|---|---|---|---|---|---|---|---|---|
| | | | | | Amino acids | | | |
| 1 | Leucine | 1.16 | 1.49 | 5.91 | 86, 75, 73, 103, 61, 146, 188 | 86 | 1 | MS |
| 2 | Valine | 0.95 | 1.29 | 6.56 | 144, 73, 147, 45, 218, 100, 59, 133, 103 | 218 | 2 | MS |
| 3 | Isoleucine | 1.19 | 1.28 | 7.33 | 73, 158, 75, 117, 147, 45, 218, 100, 133, 130 | 158 | 2 | MS |
| 4 | Proline | 1.73 | 1.36 | 7.38 | 142, 73, 45, 143, 59, 216, 100, 133 | 142 | 2 | MS |
| 5 | Glycine | 1.26 | 1.61 | 7.46 | 73, 174, 147, 86, 45, 100, 59, 175, 248, 133, 75, | 174 | 3 | MS |
| 6 | Serine | 1.55 | 1.56 | 7.96 | 73, 100, 188, 147, 45, 204, 59, 114, 133, 218, 262 | 204 | 3 | MS |
| 7 | Threonine | 1.22 | 1.21 | 8.21 | 73, 57, 117, 101, 219, 218, 45, 147, 100, 129, 133, 291 | 219 | 3 | MS |
| 8 | Aspartic acid | 0.08 | 1.25 | 8.51 | 73, 160, 75, 130, 117, 116, 45, 147, 100, 245, 234, 202 | 160 | 2 | MS |
| 9 | Pyroglutamic acid | 2.55 | 2.02 | 9.40 | 156, 73, 147, 45, 230, 258 | 156 | 2 | MS |
| 10 | GABA | 1.37 | 1.14 | 9.42 | 73, 156, 174, 147, 45, 86, 59, 304, 216, 246 | 174 | 3 | MS |
| 11 | Glutamic acid | 1.78 | 1.38 | 10.13 | 73, 246, 75, 128, 147, 84, 156, 45, 56, 230, 100 | 246 | 3 | MS |
| 12 | Phenylalanine | 1.42 | 1.45 | 10.23 | 73, 218, 192, 100, 45, 147, 59, 133, 266, | 218 | 2 | MS |
| | | | | | Organic acids | | | |
| 13 | Propanoic acid | 1.08 | 1.90 | 7.69 | 73, 147, 189, 133, 45, 102, 103, 117, 292, 205 | 189 | 3 | MS |
| 14 | Fumaric acid | 2.25 | 1.90 | 7.78 | 147, 73, 245, 75, 99, 45, 241, 133, 113, | 245 | 2 | MS |
| 15 | Malic acid | 2.23 | 1.72 | 9.08 | 73, 147, 75, 45, 133, 55, 233, 101, 189, 245, 117 | 233 | 3 | MS |
| 16 | Citric acid | 1.34 | 1.04 | 11.66 | 73, 147, 273, 45, 211, 133, 183, 347, 375, 257 | 273 | 4 | MS |
| 17 | Gluconic acid | 0.51 | 1.34 | 12.96 | 73, 147, 217, 103, 75, 205, 45, 129, 117, 333, 292, 133 | 333 | 6 | MS |
| | | | | | Fatty acids | | | |
| 18 | Palmitic acid | 1.07 | 1.23 | 13.10 | 73, 75, 117, 129, 147, 132, 217, 45, 55, 131, 205 | 129 | 1 | MS |
| 19 | Linoleic acid | 0.92 | 1.15 | 14.06 | 73, 75, 67, 81, 129, 55, 117, 80 95, 337 | 337 | 1 | MS |
| 20 | Oleic acid | 0.67 | 1.69 | 14.08 | 73, 75, 117, 129, 55, 67, 81, 96, 145, 217, 339 | 339 | 1 | MS |
| | | | | | Sugars & sugar alcohols | | | |
| 21 | Glycerol | 1.39 | 1.40 | 7.14 | 73, 147, 117, 103, 205, 133, 218, 299 | 191 | 3 | MS |
| 22 | Erythritol | 1.25 | 1.02 | 9.27 | 73, 147, 217, 103, 117, 205, 133, 189, 277, 307 | 277 | 4 | MS |
| 23 | Xylose | 0.64 | 0.91 | 10.54 | 73, 103, 147, 45, 75, 307, 133, 117, 189, 129, 59, 89 | 103 | 4 | MS |
| 24 | Xylitol | 1.32 | 1.37 | 10.97 | 73, 147, 217, 103, 129, 117, 205, 133, 45, 189, 319 | 217 | 5 | MS |
| 25 | Fructose | 1.33 | 1.58 | 12.09 | 73, 103, 217, 147, 133, 307, 45, 117, 89, 189 | 103 | 5 | MS/STD |
| 26 | Glucose | 1.28 | 1.03 | 12.33 | 73, 147, 205, 160, 103, 319, 217, 157, 117 | 103 | 5 | MS/STD |
| 27 | myo-Inositol | 2.29 | 1.94 | 13.51 | 73, 147, 217, 305, 191, 129, 133, 318, 103, 45, 204 | 305 | 6 | MS/STD |
| 28 | Glyceryl-glycoside | 0.09 | 1.69 | 14.70 | 73, 204, 147, 103, 205, 129, 217, 117, 133, 337, 169, 191 | 337 | 6 | MS |
| 29 | Sucrose | 0.22 | 1.22 | 16.58 | 73, 361, 147, 217, 103, 169, 129, 271, 191, 437, 319 | 157 | 8 | MS |
| 30 | Lactose | 0.78 | 0.85 | 17.17 | 73, 147, 204, 103, 217, 361, 129, 361, 319, 480 | 361 | 8 | MS/STD |
| 31 | Maltose | 1.81 | 1.58 | 17.49 | 73, 204, 147, 217, 103, 129, 361, 133, 117, 169, 319 | 204 | 8 | MS/STD |

[a] Tentatively identified metabolites were selected as differential variables based on *p*-value < 0.05 and VIP 1, 2 > 0.7; VIP 1 and VIP 2, value of variable importance in projection from PLS1 and PLS2 of PLS-DA model, respectively (Figure 3). [b] $t_R$, Retention time. [c] *m*/*z*, the selected ion for identification. [d] TMS, trimethylsilyl. [e] ID, identification. STD, standard compounds; MS, the mass spectra of NIST and in-house libraries.

**Table S2**. List of identified secondary metabolites selected as variables according to different cereal grains and hot peppers used in gochujang by using UHPLC-LTQ-IT-MS/MS data set.

| No. | Tentative Metabolites [a] | $t_R$ (min) | Measured Mass (*m*/*z*) | Adducts | $MS^n$ Fragments (*m*/*z*) [b] | M.W. | $\lambda_{max}$ (nm) | ID [c] |
|---|---|---|---|---|---|---|---|---|
| | | | | Flavonoids | | | | |
| 32 | Apigenin-*C*-hexoside-*C*-pentoside [d] | 6.91 | 565 | $[M + H]^+$ | **565** > **547** > **529**, 511, 499, 469, 457, 451 | 564 | 200, 270 | [1] |
| 33 | Luteolin-*O*-apiosyl-glucoside [f] | 7.51 | 581 | $[M + H]^+$ | **581** > 449, **287**, 256 > 245 | 580 | 268, 287, 321, 366 | [1,2] |
| 34 | Luteolin-*C*-hexoside [d,f] | 7.68 | 449 | $[M + H]^+$ | **449** > 432, **287** | 448 | 266, 283, 366, 414, 586 | [1,2] |
| 35 | Genistin [f] | 7.82 | 433 | $[M + H]^+$ | **433** > 415, **271** > 254, 243, 216, 154 | 432 | 200, 260 | [3] |
| 36 | Apigenin-*O*-apiosyl-glucoside [e,f] | 8.05 | 565 | $[M + H]^+$ | **565** > 433, **271** > 229, 154, 191 | 564 | 267, 335, 423 | [4], Lib. |
| 37 | Quercetin-*O*-rhamnoside [d] | 8.22 | 449 | $[M + H]^+$ | **449** > **303**, 287 > 285, 205, 165, 144 | 448 | 252, 286, 366 | [1], STD |
| 38 | Apigenin-*O*-glucoside [f] | 8.29 | 433 | $[M + H]^+$ | **433** > **271**, 154 > 253, 125 | 432 | 270 | Lib., STD |
| 39 | Hydroxydaidzein [d,f] | 8.97 | 271 | $[M + H]^+$ | **271** > **225** > 207,**197** > **141**,**129**, 113, 86 | 270 | 202, 269 | [5], Lib. |
| 40 | Genistein-*O*-di-hexoside [d,e] | 9.37 | 595 | $[M + H]^+$ | **595** > **433** > **289** > **271**, 253, 243, 225 | 594 | 204, 270 | [3] |
| 41 | Daidzein [e,f] | 9.46 | 255 | $[M + H]^+$ | **255** > 255, 237, 228 | 254 | 203, 268 | [3] |
| 42 | Glycitein [e,f] | 9.67 | 285 | $[M + H]^+$ | **285** > 267, 257, 240 | 284 | 202, 271 | [3] |
| 43 | Luteolin [f] | 9.78 | 287 | $[M + H]^+$ | **287** > 269, 229, 199 | 286 | 209, 345, 420 | Lib. |
| 44 | Genistein [e,f] | 10.64 | 271 | $[M + H]^+$ | **271** > 253, 215, 175, 153 | 270 | 289, 326, 366 | [3] |
| | | | | Soyasaponins | | | | |
| 45 | Soyasaponin V [e,f] | 11.36 | 959 | $[M + H]^+$ | **959** > 797, 635, **617** > **599**, 581, 441, 423 | 958 | 215 | [6] |
| 46 | Soyasaponin I [e,f] | 11.54 | 943 | $[M + H]^+$ | **943** > **797**, 781 > 635, 617, **599** > 581, 441, 423, 351 | 942 | 216 | [6] |
| 47 | Soyasaponin II [e,f] | 11.86 | 913 | $[M + H]^+$ | **913** > 895, 781, 767, 617, 605, 441 | 912 | 217 | [6] |
| 48 | Soyasaponin III [e,f] | 11.95 | 797 | $[M + H]^+$ | **797** > 635, 617, **599** > **581**, 441, 423 > 405, 353, 350, 201 | 796 | 217, 287 | [6] |
| | | | | Capsaicinoids & capsinoids | | | | |
| 49 | Dihydrocapsiate [d,e,f] | 9.99 | 309 | $[M + H]^+$ | **309** > **291** > 281, **263** > 236, 207 | 308 | 297, 321, 366 | [7] |
| 50 | Nordihydrocapsaicin [e,f] | 13.13 | 294 | $[M + H]^+$ | **294** > 170, **137** > 122, **109**, 91, 81 > 107, 94, 91, **81** | 293 | 218, 280, 366, 377 | [8] |
| 51 | Capsaicin [e,f] | 13.29 | 306 | $[M + H]^+$ | **306** > **137**, 170, 182, 289 > 122, 109 | 305 | 218, 281, 366, 377 | [8] |
| 52 | Dihydrocapsaicin [d,e,f] | 14.03 | 308 | $[M + H]^+$ | **308** > 184, **137** > 122, 109, 91, 81 | 307 | 203, 218, 280 | [8] |
| | | | | Lipids | | | | |
| 53 | Pinellic acid [d] | 10.83 | 353 | $[M + Na]^+$ | **353** > 335 > 317, 289, 277, 261, 207, 167 | 330 | 213, 265, 334, 366 | [9] |
| 54 | LysoPC 14:0 [d] | 13.47 | 468 | $[M + H]^+$ | - | 467 | 218 | [10] |
| 55 | LysoPC 14:0 [d,f] | 13.74 | 468 | $[M + H]^+$ | **468** > **450**, 184 > **391**, 268, 255, 181, 163 | 467 | 218 | [10] |
| 56 | LysoPC 18:3 [d,f] | 13.89 | 518 | $[M + H]^+$ | **518** > **500**, 184 > **441**, 305, 288, 182, 160 | 517 | 219 | [10] |
| 57 | LysoPE 18:2 [d,f] | 14.20 | 478 | $[M + H]^+$ | **478** > 460, **337** > 319, **263**, 245, 189, 175, 133, 121, 109 | 477 | 219 | [10] |
| 58 | LysoPE 18:2 [d,f] | 14.46 | 478 | $[M + H]^+$ | **478** > **460**, 337 > 417, 306, **263**, 155 > **245**, 165, 149, 137 | 477 | 219, 376 | [10] |
| 59 | LysoPC 18:2 [d,f] | 14.58 | 520 | $[M + H]^+$ | **520** > **502**, 184 > 443 | 519 | 220 | [11] |
| 60 | LysoPC 18:2 [d,f] | 14.87 | 520 | $[M + H]^+$ | **520** > **502**, 184 > 443 | 519 | 219, 278 | [11] |
| 61 | LysoPE 16:0 [e,f] | 15.14 | 454 | $[M + H]^+$ | **454** > **436**, 313 > 418, **393**, 282 > 239, **155** | 453 | 220 | [10] |
| 62 | LysoPC 16:0 [d,f] | 15.41 | 496 | $[M + H]^+$ | **496** > **478**, 184 > 419 | 495 | 220 | [11] |
| 63 | LysoPC 16:0 [d,e,f] | 15.79 | 496 | $[M + H]^+$ | **496** > 478, 184 > 419 | 495 | 220 | [11] |
| 64 | LysoPC 18:1 [d,f] | 15.95 | 522 | $[M + H]^+$ | - | 521 | 220 | [11] |
| 65 | LysoPC 18:1 [d,f] | 16.35 | 522 | $[M + H]^+$ | **522** > **504**,184 > 445, 163 | 521 | 220 | [11] |
| 66 | Linoleic ethanolamide [d] | 17.15 | 324 | $[M + H]^+$ | **324** > 307, 263, 245 > 289, 245, 175, 109 | 323 | 221 | [12] |

[a] Tentative metabolites were identified by comparing retention time ($t_R$), fragment pattern ($MS^n$), molecular weight (M.W.), and $\lambda_{max}$ (nm) with reference. [b] Numbers in bold mean major peak in the MS spectrum. [c] ID, Identification; STD, standard compounds; Ref., reference; Lib., in-house libraries. [d] Selected metabolites as variables according to different cereal grains in PLS-DA score plot (Figure 3B). [e] Significantly different metabolites between RbG-CA and RbG-CAY were selected based on *p*-value < 0.05 and VIP > 1 derived from OPLS-DA score plot (Figure 4). [f] Significantly different metabolites between RwG-CA and RwG-CF were selected based on *p*-value < 0.05 and VIP > 1 derived from OPLS-DA score plot (Figure 4).

**Table S3.** Relative contents of significantly different metabolites according to different cereal grains used in commercial gochujang.

| No. | Tentative Metabolites # | Relative contents ** (Mean ± SD × $10^4$ ) | | |
|---|---|---|---|---|
| | | WG | RbG | RwG |
| | Amino acids | | | |
| 1 | Leucine | 5.23 ± 2.32 $^{a}$ | 2.29 ± 0.39 $^{b}$ | 3.34 ± 1.20 $^{c}$ |
| 2 | Valine | 1.60 ± 0.85 $^{a}$ | 0.77 ± 0.18 $^{b}$ | 1.08 ± 0.39 $^{b}$ |
| 3 | Isoleucine | 7.22 ± 4.03 $^{a}$ | 3.32 ± 1.12 $^{b}$ | 4.32 ± 1.65 $^{b}$ |
| 4 | Proline | 32.21 ± 14.1 $^{a}$ | 19.89 ± 6.39 $^{b}$ | 17.38 ± 5.07 $^{b}$ |
| 5 | Glycine | 14.69 ± 6.45 $^{a}$ | 5.76 ± 0.83 $^{b}$ | 8.92 ± 3.08 $^{c}$ |
| 6 | Serine | 5.63 ± 2.79 $^{a}$ | 1.99 ± 0.5 4 $^{b}$ | 2.75 ± 1.18 $^{b}$ |
| 7 | Threonine | 1.42 ± 0.77 $^{a}$ | 0.72 ± 0.27 $^{b}$ | 0.85 ± 0.34 $^{b}$ |
| 8 | Aspartic acid | 1.12 ± 0.22 $^{a}$ | 0.75 ± 0.18 $^{b}$ | 1.10 ± 0.43 $^{a}$ |
| 9 | Pyroglutamic acid | 59.17 ± 10.5 $^{a}$ | 24.78 ± 6.20 $^{b}$ | 19.83 ± 8.65 $^{b}$ |
| 10 | GABA | 3.70 ± 0.79 $^{a}$ | 4.26 ± 0.22 $^{a}$ | 5.12 ± 1.53 $^{b}$ |
| 11 | Glutamic acid | 8.39 ± 4.81 $^{a}$ | 4.03 ± 1.81 $^{b}$ | 2.84 ± 2.43 $^{b}$ |
| 12 | Phenylalanine | 4.53 ± 2.64 $^{a}$ | 1.51 ± 0.70 $^{b}$ | 2.17 ± 1.02 $^{b}$ |
| | Organic acids | | | |
| 13 | Propanoic acid | 0.86 ± 0.07 $^{a}$ | 0.99 ± 0.18 $^{b}$ | 0.74 ± 0.09 $^{c}$ |
| 14 | Fumaric acid | 0.21 ± 0.05 $^{a}$ | 0.18 ± 0.02 $^{b}$ | 0.12 ± 0.02 $^{c}$ |
| 15 | Malic acid | 2.24 ± 0.52 $^{a}$ | 1.71 ± 0.26 $^{b}$ | 1.37 ± 0.23 $^{c}$ |
| 16 | Citric acid | 41.88 ± 10.7 $^{a}$ | 31.82 ± 6.98 $^{b}$ | 29.50 ± 10.8 $^{b}$ |
| 17 | Gluconic acid | 2.20 ± 1.90 $^{a}$ | 0.55 ± 0.15 $^{b}$ | 1.55 ± 0.75 $^{a}$ |
| | Fatty acids | | | |
| 18 | Palmitic acid | 13.18 ± 5.39 $^{a}$ | 11.95 ± 2.80 $^{a}$ | 19.17 ± 8.54 $^{b}$ |
| 19 | Linoleic acid | 0.12 ± 0.06 $^{a}$ | 0.14 ± 0.08 $^{a}$ | 0.08 ± 0.05 $^{b}$ |
| 20 | Oleic acid | 0.04 ± 0.02 $^{a}$ | 0.07 ± 0.03 $^{b}$ | 0.03 ± 0.02 $^{a}$ |
| | Sugars & sugar alcohols | | | |
| 21 | Glycerol | 14.76 ± 0.56 $^{a}$ | 14.74 ± 0.74 $^{a}$ | 13.65 ± 1.05 $^{b}$ |
| 22 | Erythritol | 0.30 ± 0.20 $^{a}$ | 0.24 ± 0.11 $^{ab}$ | 0.16 ± 0.09 $^{b}$ |
| 23 | Xylose | 8.21 ± 1.96 $^{a}$ | 5.46 ± 1.00 $^{b}$ | 6.57 ± 3.23 $^{ab}$ |
| 24 | Xylitol | 31.83 ± 14.0 $^{a}$ | 32.04 ± 8.57 $^{a}$ | 19.46 ± 9.90 $^{b}$ |
| 25 | Fructose | 243.81 ± 16.5 $^{a}$ | 250.62 ± 6.73 $^{a}$ | 219.28 ± 26.0 $^{b}$ |
| 26 | Glucose | 66.86 ± 2.82 $^{a}$ | 70.40 ± 1.65 $^{ab}$ | 74.69 ± 9.45 $^{b}$ |
| 27 | myo-Inositol | 7.00 ± 1.07 $^{a}$ | 6.12 ± 0.78 $^{b}$ | 4.54 ± 0.77 $^{c}$ |
| 28 | Glyceryl-glycoside | 1.47 ± 0.79 $^{a}$ | 0.44 ± 0.26 $^{b}$ | 1.30 ± 0.54 $^{a}$ |
| 29 | Sucrose | 0.20 ± 0.24 $^{a}$ | 1.10 ± 1.70 $^{b}$ | 0.14 ± 0.11 $^{a}$ |
| 30 | Lactose | 42.46 ± 4.52 $^{a}$ | 45.76 ± 2.77 $^{b}$ | 44.90 ± 2.84 $^{b}$ |
| 31 | Maltose | 1.91 ± 0.76 $^{a}$ | 2.70 ± 0.58 $^{a}$ | 4.74 ± 2.08 $^{b}$ |
| | Flavonoids | | | |
| 32 | Apigenin-*C*-hexoside-*C*-pentoside | 1.23 ± 0.91 $^{a}$ | 0.20 ± 0.77 $^{b}$ | 0.40 ± 0.89 $^{b}$ |
| 34 | Luteolin-*C*-hexoside | 2.21 ± 1.71 $^{a}$ | 3.70 ± 1.81 $^{b}$ | 2.85 ± 1.30 $^{ab}$ |
| 37 | Quercetin-*O*-rhamnoside | 3.71 ± 1.87 $^{a}$ | 5.18 ± 1.69 $^{b}$ | 3.29 ± 1.40 $^{a}$ |
| 39 | Hydroxydaidzein | 1.53 ± 0.55 $^{a}$ | 0.16 ± 0.25 $^{b}$ | 0.86 ± 1.10 $^{c}$ |
| 40 | Genistein-*O*-di-hexoside | 1.70 ± 1.58 $^{a}$ | 3.20 ± 2.11 $^{a}$ | 8.19 ± 5.15 $^{b}$ |

| | | | | |
|---|---|---|---|---|
| | Capsaicinoids & capsinoids | | | |
| 49 | Dihydrocapsiate | 43.66 ± 58.7 [a] | 11.60 ± 5.00 [b] | 14.19 ± 12.2 [b] |
| 52 | Dihydrocapsaicin | 109.28 ±17.2[a] | 136.62 ± 18.5 [b] | 150.82 ± 47.4 [b] |
| | lipids | | | |
| 53 | Pinellic acid | 3.18 ±1.04 [a] | 3.24 ± 0.42 [a] | 3.72 ± 0.48 [b] |
| 54 | LysoPC 14:0 | 0.08 ± 0.14 [a] | 1.11 ± 0.47 [b] | 0.25 ± 0.23 [a] |
| 55 | LysoPC 14:0 | 1.29 ± 1.83[a] | 14.84 ± 6.28 [b] | 3.27 ± 3.29 [a] |
| 56 | LysoPC 18:3 | 2.13 ± 0.99 [a] | 2.53 ± 0.67 [a] | 0.63 ± 0.43 [b] |
| 57 | LysoPE 18:2 | 3.94 ±4.33[a] | 2.20 ± 0.31[b] | 1.00 ± 0.56 [b] |
| 58 | LysoPE 18:2 | 5.85 ± 3.42 [a] | 13.02 ± 2.56 [b] | 3.86 ± 2.92 [a] |
| 59 | LysoPC 18:2 | 10.65 ± 10.2 [a] | 7.08 ± 1.51 [b] | 2.47 ± 1.50 [c] |
| 60 | LysoPC 18:2 | 41.41 ± 28.8 [a] | 70.30 ±16.2 [b] | 19.47 ± 15.6 [c] |
| 62 | LysoPC 16:0 | 4.23 ± 3.34 [a] | 10.61 ± 3.89 [b] | 4.20 ± 3.01 [a] |
| 63 | LysoPC 16:0 | 33.99 ± 32.7 [a] | 91.76 ± 27.9 [b] | 34.57 ± 31.0 [a] |
| 64 | LysoPC 18:1 | 2.55 ± 1.76 [a] | 2.08 ± 0.74 [a] | 1.09 ± 0.61 [b] |
| 65 | LysoPC 18:1 | 8.07 ± 7.12 [a] | 16.17 ± 6.54 [b] | 5.89 ±5.98 [a] |
| 66 | Linoleic ethanolamide | 66.22 ± 14.5 [a] | 13.13 ± 3.80 [b] | 24.87 ± 17.7 [c] |

[a,b,c] Different letters indicate significant differences calculated by Duncan's multiple comparison test ($p$-value < 0.05). [#] Tentative identified metabolites were selected as variables based on variable importance in projection (VIP > 0.7) from PLS-DA and $p$-value < 0.05. [**] Relative contents; values are means of relative peak areas in triplicate from alignment data ± standard deviation (SD); WG, wheat gochujang; RbG, brown rice gochujang; RwG, white rice gochujang.

## References


1. Wahyuni, Y.; Ballester, A.R.; Sudarmonowati, E.; Bino, R.J.; Bovy, A.G. Metabolite biodiversity in pepper (*Capsicum*) fruits of thirty-two diverse accessions: Variation in health-related compounds and implications for breeding. *Phytochem.* **2011**, *72*, 1358–1370.
2. Jeong, W.Y.; Jin, J.S.; Cho, Y.A.; Lee, J.H.; Park, S.; Jeong, S.W.; Kim, Y.H.; Lim, C.S.; Abd El-Aty, A.M.; Kim, G.S.; et al. Determination of polyphenols in three *Capsicum annuum* L. (bell pepper) varieties using high-performance liquid chromatography-tandem mass spectrometry: Their contribution to overall antioxidant and anticancer activity. *J. Sep. Sci.* **2011**, *34*, 2967–2974.
3. Cavaliere, C.; Cucci, F.; Foglia, P.; Guarino, C.; Samperi, R.; Laganà, A. Flavonoid profile in soybeans by high-performance liquid chromatography/tandem mass spectrometry. *Rapid Commun. Mass Spectrom.* **2007**, *21*, 2177–2187.
4. Li, P.; Jia, J.; Zhang, D.; Xie, J.; Xu, X.; Wei, D. In vitro and in vivo antioxidant activities of a flavonoid isolated from celery (*Apium graveolens* L. var. dulce). *Food Funct.* **2014**, *5*, 50–56.
5. Lee, S.; Seo, M.H.; Oh, D.K.; Lee, C.H. Targeted metabolomics for *Aspergillus oryzae*-mediated biotransformation of soybean isoflavones, showing variations in primary metabolites. *Biosci. Biotechnol. Biochem.* **2014**, *78*, 167–174.
6. Lee, S.Y.; Lee, S.; Lee, S.; Oh, J.Y.; Jeon, E.J.; Ryu, H.S.; Lee, C.H. Primary and secondary metabolite profiling of doenjang, a fermented soybean paste during industrial processing. *Food Chem.* **2014**, *165*, 157–166.
7. Singh, S.; Jarret, R.; Russo, V.; Majetich, G.; Shimkus, J.; Bushway, R.; Perkins, B. Determination of capsinoids by HPLC-DAD in *Capsicum* species. *J. Agric. Food Chem.* **2009**, *57*, 3452–3457.
8. Choi, S.H.; Suh, B.S.; Kozukue, E.; Kozukue, N.; Levin, C.E.; Friedman, M. Analysis of the contents of pungent compounds in fresh Korean red peppers and in pepper-containing foods. *J. Agric. Food Chem.* **2006**, *54*, 9024–9031.
9. Kim, G.R.; Jung, E.S.; Lee, S.; Lim, S.H.; Ha, S.H.; Lee, C.H. Combined mass spectrometry-based metabolite profiling of different pigmented rice (*Oryza sativa* L.) seeds and correlation with antioxidant activities. *Molecules* **2014**, *19*, 15673–15686.
10. Fang, N.; Yu, S.; Badger, T.M. LC-MS/MS analysis of lysophospholipids associated with soy protein isolate. *J. Agric. Food Chem.* **2003**, *51*, 6676–6682.

11. Zaima, N.; Yoshimura, Y.; Kawamura, Y.; Moriyama, T. Distribution of lysophosphatidylcholine in the endosperm of *Oryza sativa* rice. *Rapid Commun. Mass Spectrom.* **2014**, *28*, 1515–1520.
12. Palandra, J.; Prusakiewicz, J.; Ozer, J.S.; Zhang, Y.; Heath, T.G. Endogenous ethanolamide analysis in human plasma using HPLC tandem MS with electrospray ionization. *J. Chromatogr. B* **2009**, *877*, 2052–2060.