

Supplementary Materials

Table S1. List of tentatively identified secondary metabolites of nine different Korean species of rice seeds using UPLC-Q-TOF-MS.

Tentative Identification ^a	UPLC-Q-TOF-MS					LC-ESI-MS/MS				
	RT ^b (min)	Measured Mass (<i>m/z</i>)		Elemental Composition (Formular)	Δ ppm	iFit	MS ⁿ Fragments (<i>m/z</i>)	Adduct	λ_{\max}	Ref. ^c
Cyanidin-3-glucoside	3.11	447.09	449.108	C ₂₁ H ₂₁ O ₁₁	-3.3	0.11	449 > 287 > 213 (+)	[M+H] ⁺	277, 515	std ^d
Peonidin-3-glucoside	3.35	461.108	463.127	C ₂₂ H ₂₃ O ₁₁	2.6	0.72	463 > 301 > 286 (+)	[M+H] ⁺	276, 517	std
Pronathocyanidin dimer	3.1	577.133	579.153	C ₃₀ H ₂₇ O ₁₂	5.2	1.96	579 > 453 > 301(+)	[M+H] ⁺	241, 278	[6,45]
Proanthocyanidin trimer	3.14	865.191	867.218	C ₄₅ H ₃₉ O ₁₈	1.4	3.06	865 > 695 > 543 (-)	[M-H] ⁻	242, 277	[6,45]
Catechin *	3.23	289.071	291.093	C ₁₅ H ₁₃ O ₆	2.1	0.84	289 > 253 > 203 (-)	[M-H] ⁻	241, 277	std
Apigenin-6- <i>C</i> -glucosyl-8- <i>C</i> -arabinoside	3.64	563.138	565.164	C ₂₆ H ₂₇ O ₁₄	0.4	0.51	563 > 473 > 383 (-)	[M-H] ⁻	273, 308	[27,28]
Tricin- <i>O</i> -rhamnoside- <i>O</i> -hexoside	4.18	637.172	639.199	C ₂₉ H ₃₅ O ₁₆	6.3	2.4	639 > 493 > 331 (+)	[M+H] ⁺	272, 313	[29]
Pinellic acid	5.82	329.233	353.232	C ₁₈ H ₃₃ O ₅	-7.6	0.03	329 > 311,229,171 > 293 (-)	[M-H] ⁻	231, 313	[30]
LysoPC 14:0	7.71	512.297	468.312	C ₂₃ H ₄₇ NO ₉ P	2	1.08	512 > 452 > 227 (-)	[M+FA-H] ⁻	239, 264	[43,44]
LysoPC 18:2	8.28	564.334	520.343	C ₂₇ H ₅₁ NO ₉ P	-1.9	2.44	564 > 504 > 279 (-)	[M+FA-H] ⁻	239, 271	[43,44]
LysoPC 16:0	8.75	480.31	496.342	C ₂₄ H ₅₁ NO ₇ P	2	0.16	496 > 184 > 86 (+)	[M+CH ₃] ⁺	241, 304	[43,44]
LysoPC 18:1	8.98	566.346	522.359	C ₂₇ H ₅₃ NO ₉ P	-3	0.18	566 > 506 > 281 (-)	[M+FA-H] ⁻	237, 273	[43,44]

^a Identified metabolites based on VIP > 0.7, and a *p*-value < 0.05 from the PLS-DA model. ^b Retention time. ^c Reference. ^d Standard compound. * Target identified.

Table S2. Significantly different primary metabolites identified from nine different species of rice seeds extracts using GC-TOF-MS.

RT ^a (min)	Metabolites ^b	MS Fragment Ions (<i>m/z</i>)	Ref. ^c
<i>Amino acids</i>			
6.44	Valine	73-144-75-147-59-74-100-218-145-58	STD
7.24	Proline	73-174-86-147-59-100-75-133-74-175	STD
7.81	Serine	73-57-117-75-101-147-74-219-218-59	STD
8.05	Threonin	73-147-75-55-74-59-133-101-148-233	STD
9.2	Aspartic acid	73-156-174-75-147-86-59-74-100-175	STD
9.26	GABA	73-147-75-220-59-100-218-74-84-55	STD
9.97	Glutamic acid	73-218-75-192-147-74-59-91-58	STD
10.06	Phenylalanine	73-75-103-116-147-74-132-100-59-217	STD
10.4	Asparagine	73-103-147-217-129-74-117-75-133-205	STD
14.06	Tryptophan	73-202-75-131-74-203-116-59-100-55	STD
16.29	Adenosine	73-129-75-103-74-217-147-230-236-55	STD
<i>Organic acid</i>			
7.03	Pyruvate	73-142-75-117-147-59-78-74-180-57	STD
7.21	Nicotinic acid	73-142-75-147-59-143-74-72-66-58	STD
7.34	Succinic acid	73-100-204-218-75-147-59-74-188-116	STD
7.63	Maleic acid	73-147-75-245-100-74-143-59-83-148	STD
8.92	Malonic acid	73-100-147-232-75-74-117-59-156-133	STD
9.13	Salicylic acid	73-267-75-91-135-74-77-149-268-209	STD
11.5	Citric acid	73-103-147-217-75-74-59-89-129-133	STD
<i>Sugar & Sugar alcohols</i>			
0.37	Xylose	73-116-75-74-132-147-100-141-59-188	STD
10.71	Xylitol	73-103-147-217-129-117-74-75-205-133	STD
11.9	Fructose	73-147-103-160-74-75-129-117-205-217	STD
11.97	Fructose	73-103-147-217-74-75-133-59-117-89	STD
12.22	Glucose	73-202-75-131-74-203-116-59-100-55	STD
12.77	Gluconic acid	73-147-103-74-117-75-217-205-133-129	STD
13.34	myo-inositol	73-147-217-191-103-129-74-133-75-318	STD
16.43	Sucrose	73-103-147-217-129-74-75-169-117-361	STD
16.86	Maltose	73-75-147-103-217-129-74-59-361-204	STD

^a Retention time; ^b Identified metabolites basend on VIP > 0.7 and a *p*-value < 0.05 from the PLS-DA model; ^c Standard compound.