

Appendix B. The other metabolites involved in differential metabolite pathways

Metabolites	Formula	Ratio	P. value	KEGG.ID	Pathway
WGBR vs. rice (positive ions)					
Phenylpyruvic acid	C ₉ H ₈ O ₃	2.9751	0.0453	C00166	Phenylalanine, tyrosine and tryptophan biosynthesis (map00400)
Indole	C ₈ H ₇ N	11.1147	0.0445	C00463	map00400
WGBR-HTP vs. rice (positive ions)					
10-Hydroxydihydrosanguinarine	C ₂₀ H ₁₅ NO ₅	0.7917	0.0464	C05247	Isoquinoline alkaloid biosynthesis (map00950)
(S)-cis-N-Methylcanadine	C ₂₁ H ₂₄ NO ₄ ⁺	29.8522	0.0302	C02915	map00950
Demethylisoalangsoid	C ₂₄ H ₂₉ NO ₁₀	6.3294	0.0129	C11814	map00950
L-Dopa	C ₉ H ₁₁ NO ₄	2.6752	0.0337	C00355	map00950
6-O-Methyl-N-deacetylisopecoside aglycon	C ₂₀ H ₂₅ NO ₆	0.8086	0.0472	C21583	map00950
7-Deoxyloganate	C ₁₆ H ₂₄ O ₉	6.0642	0.0355	C11636	Monoterpenoid biosynthesis (map00902)
Loganate, Loganic acid	C ₁₆ H ₂₄ O ₁₀	3.7231	0.0251	C01512	map00902
(-)-Isopiperitenone	C ₁₀ H ₁₄ O	0.5891	0.0380	C02485	map00902
WGBR-T18 vs rice (positive ions)					
Diethanolamine	C ₄ H ₁₁ NO ₂	0.7187	0.0437	C06772	Glycerophospholipid metabolism (map00564)
Triethanolamine	C ₆ H ₁₅ NO ₃	6.0258	0.0460	C06771	map00564
WGBR-HTP vs Brown-rice (positive ions)					
L-Methionine	C ₅ H ₁₁ NO ₂ S	3.1593	0.0395	C00073	Cysteine and methionine metabolism (map00270)
O-Acetyl-L-homoserine, O-Acetylhomoserine	C ₆ H ₁₁ NO ₄	0.1690	0.0123	C01077	map00270
5-Methylthioadenosine	C ₁₁ H ₁₅ N ₅ O ₃ S	12.5720	0.0093	C00170	map00270
WGBR-T18 vs Brown-rice (positive ions)					
Sinapine	C ₁₆ H ₂₄ NO ₅ ⁺	7.3324	0.0472	C00933	Phenylpropanoid biosynthesis (map00940)
2-Phosphonoacetaldehyde, 2-Oxoethylphosphonate	C ₂ H ₅ O ₄ P	8.4282	0.0423	C03167	map00440
WGBR vs rice (negative ions)					
Cobalt-dihydro-precorrin 6, Cobalt-precorrin 6B	C ₄₄ H ₅₅ CoN ₄ O ₁₆ ⁺	3.2056	0.0354	C11543	Porphyrin and chlorophyll metabolism (map00860)
Heme	C ₃₄ H ₃₂ FeN ₄ O ₄	4.9926	0.0447	C00032	map00860
Bacteriochlorophyllide a	C ₃₅ H ₃₆ MgN ₄ O ₆	50.8763	0.0430	C18155	map00860
Chlorophyllide b	C ₃₅ H ₃₂ MgN ₄ O ₆	17.6772	0.0452	C16541	map00860
Uroporphyrin I	C ₄₀ H ₃₈ N ₄ O ₁₆	10.0680	0.0447	C05767	map00860
8,12-Diethyl-3-vinylbacteriochlorophyllide d	C ₃₄ H ₃₄ MgN ₄ O ₃	3.4540	0.0432	C21427	map00860
Bacteriochlorophyllide b	C ₃₅ H ₃₄ MgN ₄ O ₆	0.2794	0.0391	C18156	map00860

Mesaconic acid	C ₅ H ₆ O ₄	13.2466	0.0345	C01732	C5-Branched dibasic acid metabolism (map00660)
Trans-Aconitic acid	C ₆ H ₆ O ₆	9.1933	0.0487	C02341	map00660
WGBR-HTP vs rice (negative ions)					
P1,P4-Bis(5'-xanthosyl) tetraphosphate	C ₂₀ H ₂₆ N ₈ O ₂₃ P ₄	27.7186	0.0114	C04392	Purine metabolism (map00230)
Adenine	C ₅ H ₅ N ₅	11.1555	0.0324	C00147	map00230; Zeatin biosynthesis (map00908);
Adenosine tetraphosphate	C ₁₀ H ₁₇ N ₅ O ₁₆ P ₄	0.0737	0.0338	C03483	Purine metabolism (map00230)
Guanosine 3'-phosphate, 3'-GMP, 3'-Guanylic acid, Guo-3'-P, Gp	C ₁₀ H ₁₄ N ₅ O ₈ P	65.3504	0.0171	C06193	map00230
Inosine	C ₁₀ H ₁₂ N ₄ O ₅	10.7198	0.0383	C00294	map00230
IDP, Inosine					map00230
5'-diphosphate, Inosine diphosphate	C ₁₀ H ₁₄ N ₄ O ₁₁ P ₂	6.8062	0.0427	C00104	
Xanthosine	C ₁₀ H ₁₂ N ₄ O ₆	3.6441	0.0479	C01762	map00230
Sulfate	H ₂ O ₄ S	0.4950	0.0104	C00059	map00230
2-Descarboxy-betanidin	C ₁₇ H ₁₇ N ₂ O ₆ ⁺	7.9875	0.0329	C17757	Betalain biosynthesis (map00965)
Celosianin II	C ₄₀ H ₄₂ N ₂ O ₂₂	3.1236	0.0436	C08542	map00965
Lampranthin II	C ₃₄ H ₃₄ N ₂ O ₁₆	6.9173	0.0370	C08552	map00965
Cyclo-Dopa-glucuronylglucoside;	C ₂₁ H ₂₇ NO ₁₅	0.5778	0.0315	C17752	map00965
Magnesium protoporphyrin, Magnesium protoporphyrin IX, Mg-protoporphyrin IX	C ₃₄ H ₃₂ MgN ₄ O ₄	45.7314	0.0384	C03516	Porphyrin and chlorophyll metabolism (map00860)
Cobalt-precorrin 8	C ₄₅ H ₅₉ CoN ₄ O ₁₄ ⁺	9.2972	0.0424	C11545	map00860
Heme	C ₃₄ H ₃₂ FeN ₄ O ₄	4.6370	0.0178	C00032	map00860
Bacteriochlorophyllide a	C ₃₅ H ₃₆ MgN ₄ O ₆	30.5069	0.0175	C18155	map00860
Chlorophyllide b	C ₃₅ H ₃₂ MgN ₄ O ₆	18.8162	0.0202	C16541	map00860
Uroporphyrin I	C ₄₀ H ₃₈ N ₄ O ₁₆	12.7908	0.0145	C05767	map00860
Bacteriochlorophyllide b	C ₃₅ H ₃₄ MgN ₄ O ₆	0.5034	0.0489	C18156	map00860
CDP	C ₉ H ₁₅ N ₃ O ₁₁ P ₂	39.8860	0.0271	C00112	Pyrimidine metabolism (map00240)
Uridine	C ₉ H ₁₂ N ₂ O ₆	37.3900	0.0193	C00299	map00240
Uracil	C ₄ H ₄ N ₂ O ₂	5.9968	0.0416	C00106	map00240
Thymidine	C ₁₀ H ₁₄ N ₂ O ₅	217.2801	0.0136	C00214	map00240
Pyrophosphate	H ₄ O ₇ P ₂	38.8926	0.0233	C00013	Oxidative phosphorylation (map00190)
Flavin Mononucleotide	C ₁₇ H ₂₁ N ₄ O ₉ P	0.4836	0.0204	C00061	map00190
Cis-zeatin-7-N-glucoside	C ₁₆ H ₂₃ N ₅ O ₆	3.7672	0.0399	C16443	Zeatin biosynthesis (map00908)
Dihydrozeatin riboside monophosphate	C ₁₅ H ₂₄ N ₅ O ₈ P	0.5176	0.0134	C16445	map00908

WGBR-T18 vs rice (negative ions)

P1,P4-Bis(5'-xanthosyl) tetraphosphate	$C_{20}H_{26}N_8O_{23}P_4$	20.6462	0.0459	C04392	Purine metabolism (map00230)
Adenine	$C_5H_5N_5$	1.9040	0.0436	C00147	map00230
Inosine	$C_{10}H_{12}N_4O_5$	26.2298	0.0436	C00294	map00230
Hydroxypyruvic acid	$C_3H_4O_4$	54.1439	0.0454	C00168	Carbon metabolism (map01200); Glycine, serine and threonine metabolism (map00260) Glyoxylate and dicarboxylate metabolism (map00630)
Mesaconic acid	$C_5H_6O_4$	10.0464	0.0436	C01732	map01200; map00630
5,10-Methenyltetrahydrofolate	$C_{20}H_{22}N_7O_6^+$	7.7599	0.0436	C00445	Carbon metabolism(map01200); One carbon pool by folate (map00670)
D-Serine	$C_3H_7NO_3$	3.4263	0.0459	C00740	map00260
Hydroxymethylphosphonate, P-(Hydroxymethyl)-phosphonic acid	CH_5O_4P	8.9543	0.0274	C06455	Phosphonate and phosphinate metabolism (map00440)
alpha-D-Ribose 1,2-cyclic phosphate 5-phosphate, 5-Phospho-alpha-D-ribose 1,2-cyclic phosphate	$C_5H_{10}O_{10}P_2$	5.4861	0.0474	C20440	map00440
Chlorophyllide b	$C_{35}H_{32}MgN_4O_6$	34.8039	0.0459	C16541	Porphyrin and chlorophyll metabolism (map00860)
Uroporphyrin I	$C_{40}H_{38}N_4O_{16}$	12.7270	0.0459	C05767	map00860
8,12-Diethyl-3-vinylbacteriochlorophyllide d	$C_{34}H_{34}MgN_4O_3$	6.3209	0.0442	C21427	map00860
WGBR-HTP vs Brown-rice (negative ions)					
4-Hydroxy-4-methylglutamate	$C_6H_{11}NO_5$	0.2632	0.0395	C06034	C5-Branched dibasic acid metabolism (map00660)
Mesaconic acid	$C_5H_6O_4$	3.1221	0.0376	C01732	map00660
Trans-Aconitic acid	$C_6H_6O_6$	2.4169	0.0482	C02341	map00660
2-Hydroxyparaconate	$C_5H_6O_5$	8.4085	0.0423	C21632	map00660
Magnesium protoporphyrin; Magnesium protoporphyrin IX; Mg-protoporphyrin IX	$C_{34}H_{32}MgN_4O_4$	0.0172	0.0116	C03516	Porphyrin and chlorophyll metabolism (map00860)
Cobalt-precorrin 8	$C_{45}H_{59}CoN_4O_{14}^+$	9.6622	0.0485	C11545	map00860
Porphobilinogen	$C_{10}H_{14}N_2O_4$	11.2279	0.0435	C00931	map00860
Cobalt-precorrin 7	$C_{44}H_{57}CoN_4O_{14}$	0.3084	0.0293	C16244	map00860

+					
Chlorophyllide b	$C_{35}H_{32}MgN_4O_6$	4.7761	0.0141	C16541	map00860
8,12-Diethyl-3-vinylbacteriochlorophyllide d	$C_{34}H_{34}MgN_4O_3$	10.6862	0.0490	C21427	map00860
Bacteriochlorophyllide b	$C_{35}H_{34}MgN_4O_6$	0.4782	0.0482	C18156	map00860
P1,P4-Bis(5'-xanthosyl) tetraphosphate	$C_{20}H_{26}N_8O_{23}P_4$	2.9618	0.0400	C04392	Purine metabolism (map00230)
Adenine	$C_5H_5N_5$	3.4324	0.0123	C00147	map00230
Adenosine tetraphosphate	$C_{10}H_{17}N_5O_{16}P_4$	0.1689	0.0387	C03483	map00230
Uric acid	$C_5H_4N_4O_3$	25.5881	0.0498	C00366	map00230
Guanosine 3'-phosphate; 3'-GMP; 3'-Guanylic acid; Guo-3'-P; Gp;	$C_{10}H_{14}N_5O_8P$	9.8929	0.0364	C06193	map00230
Rhizoctin D;	$C_{17}H_{33}N_6O_7P$	2.8746	0.0297	C17961	Phosphonate and phosphinate metabolism (map00440)
Hydroxymethylphosphonate; P-(Hydroxymethyl)-phosphonic acid	CH_5O_4P	0.0568	0.0107	C06455	map00440
alpha-D-Ribose 1,2-cyclic phosphate 5-phosphate; 5-Phospho-alpha-D-ribose 1,2-cyclic phosphate;	$C_5H_{10}O_{10}P_2$	4.3423	0.0418	C20440	map00440
WGBR-T18 vs Brown-rice (negative ions)					
Glutathione disulfide					
GSSG Oxiglutatione Oxidized glutathione	$C_{20}H_{32}N_6O_{12}S_2$	0.2295	0.0441	C00127	Glutathione metabolism (map00480)
Adenine	$C_5H_5N_5$	6.0399	0.0467	C00147	Zeatin biosynthesis (map00908)
Hydroxypyruvic acid	$C_3H_4O_4$	40.5624	0.0235	C00168	Glycine, serine and threonine metabolism (map00260); Glyoxylate and dicarboxylate metabolism (map00630)
Secologanate	$C_{16}H_{22}O_{10}$	9.9704	0.0466	C01957	Monoterpenoid biosynthesis (map00902)
Uridine	$C_9H_{12}N_2O_6$	8.2010	0.0466	C00299	Pyrimidine metabolism (map00240)