

Table S1: Metabolites and Reference Standards

Acute Exercise and Fitness Status Linked to Increased Plasma Concentrations of Gut-Derived Phenolics

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Metabolite	CAS	Reference Standard	Relative Quantifier	# Transitions
theanine	3081-61-6	✓	reference standard	5
3-hydroxybenzoic acid-4-sulfate	synthetic	✓	reference standard	1
3-hydroxybenzoic acid-4-O-glucuronide	synthetic	✓	reference standard	3
hydroxybenzoic acid-diglucuronide	x	x	3-hydroxybenzoic acid-4-O-glucuronide	4
3,4-dihydroxybenzoic acid	99-50-3	✓	reference standard	3
4-hydroxybenzoic acid	99-96-7	✓	reference standard	3
4-hydroxybenzoic acid-3-O-glucuronide	synthetic	✓	reference standard	4
-(-)gallocatechin	3371-27-5	✓	reference standard	5
hippuric acid	495-69-2	✓	reference standard	3
5-hydroxyphenylpropanoic acid-3-sulfate	synthetic	✓	reference standard	1
3-methoxy-benzoic acid-4-O-glucuronide	synthetic	✓	reference standard	3
4-methoxybenzoic acid-3-sulfate	synthetic	✓	reference standard	3
2-hydroxyphenylacetic acid	614-75-5	✓	reference standard	3
hydroxybenzaldehyde-glucuronide	x	x	3-hydroxybenzoic acid-4-O-glucuronide	5
4-hydroxybenzaldehyde	123-08-0	✓	reference standard	3
hydroxyphenylacetic acid-glucuronide	x	x	4-hydroxyphenylproprionic acid-3-O-glucuronide	4
5-O-caffeoylquinic acid	x	x	4-O Caffeoylquinic acid	4
3-methoxybenzoic acid-sulfoglucuronide	x	x	3-methoxy-benzoic acid-4-O-glucuronide	4
3-methoxy-benzoic acid-4-sulfate	synthetic	✓	reference standard	3
4-methoxy-cinnamic acid-3-sulfate	synthetic	✓	reference standard	1
(+)-catechin-O-glucuronide	x	x	quercetin-3-O-glucuronide	5
(+)-catechin	7295-85-4	✓	reference standard	4
(4R)-5-(3',4'-Dihydroxyphenyl)-γ-valerolactone-4'-O-sulfate	x	✓	reference standard	4
3-O-caffeoylquinic acid	x	x	4-O-caffeoylquinic acid	4
3-(4-hydroxy-3-methoxyphenyl)propanoic acid-4-O-glucuronide	86321-28-0	✓	reference standard	1
4-methoxycinnamic acid-3-sulfoglucuronide	x	x	3-(3-hydroxy-4-methoxyphenyl)propionic acid	5
4-O-caffeoylquinic acid	905-99-7	✓	reference standard	1

phenyl-valerolactone-sulfoglucuronide	synthetic	x	3-hydroxybenzoic acid-4-O-glucuronide	5
3-hydroxy-4-methoxybenzaldehyde	621-59-0	✓	reference standard	3
4-hydroxy-3-methoxybenzoic acid	121-34-6	✓	reference standard	7
3-hydroxy-4-methoxy-cinnamic acid-3-O-glucuronide	1065272-10-7	✓	reference standard	5
3-(3-hydroxyphenyl)propionic acid	621-54-5	✓	reference standard	3
phenyl-valerolactone-sulfate	synthetic	x	3,4-dihydroxybenzoic acid	3
3,4-dihydroxybenzoic acid methyl ester	2150-43-8	✓	reference standard	4
5-(3'-hydroxyphenyl)-gamma-valerolactone-4'-O-glucuronide	synthetic	x	3-hydroxybenzoic acid-4-O-glucuronide	6
3-hydroxy-4-methoxybenzaldehyde	645-08-9	✓	reference standard	3
3-(4-hydroxyphenyl)propionic acid	501-97-3	✓	reference standard	3
-(-)epicatechin	490-46-0	✓	reference standard	5
4-hydroxycinnamic acid	7400-08-0	✓	reference standard	3
3-O-caffeoylquinic acid-O-glucuronide	x	x	3-hydroxycinnamic acid-4-O-glucuronide	6
-(-)epicatechin-O-glucuronide	x	x	quercetin-3-O-glucuronide	6
2-hydroxybenzoic acid	69-72-7	✓	reference standard	3
-(-)epigallocatechin	970-74-1	✓	reference standard	5
-(-)gallocatechin-O-glucuronide	x	x	quercetin-3-O-glucuronide	6
3-(3-hydroxy-4-methoxyphenyl)propionic acid	1135-15-5	✓	reference standard	3
4-hydroxybenzoic acid methyl ester	99-76-3	✓	reference standard	3
myricetin 3-O-galactoside	15648-86-9	✓	reference standard	1
quercetin 3-glucoside	482-35-9	✓	reference standard	1
resveratrol	501-36-0	✓	reference standard	5
myricetin	529-44-2	✓	reference standard	5
3-O-feruloylquinic acid	x	x	4-O-caffeoylquinic acid	3
4-O-feruloylquinic acid	x	x	4-O-caffeoylquinic acid	3
5-O-feruloylquinic acid	x	x	4-O-caffeoylquinic acid	3
myricetin-O-glucuronide	x	x	myricetin 3-O-galactoside	6
4-methoxy-cinnamic acid-3-O-glucuronide	1065272-10-7	✓	reference standard	4
3-methylquercetin	480-19-3	✓	reference standard	4
valerolactone-disulfate	x	x	3-hydroxybenzoic acid-4-O-glucuronide	5

-(-)epigallocatechin gallate	989-51-5	✓	reference standard	4
-(-)epigallocatechin gallate-O-glucuronide	x	x	quercetin-3-O-glucuronide	5
hydroxy-methoxyphenylacetic acid-O-glucuronide	x	x	3-(4-hydroxy-3-methoxyphenyl)propanoic acid-4-O-glucuronide	5
phenylpropanoic acid-O-glucuronide	x	x	4-hydroxyphenylproprionic acid-3-O-glucuronide	5
dihydroxybenzaldehyde-sulfate	x	x	3,4-dihydroxybenzoic acid	4
trihydroxybenzaldehyde-sulfate	x	x	3,4-dihydroxybenzoic acid	4
hippuric acid-sulfate	x	x	3,4-dihydroxybenzoic acid	4
dihydroxybenzoic acid-sulfate	x	x	3,4-dihydroxybenzoic acid	4
2,4-dihydroxy benzaldehyde	95-01-2	✓	reference standard	5
Kaempferol-7-O-neohesperidoside	17353-03-6	✓	reference standard	1
4'-O-methylquercetin	synthetic	✓	reference standard	6
quercetin-3-O-glucuronide	synthetic	✓	reference standard	1
quercetin-3-sulfate	synthetic	✓	reference standard	7
(-)-5-(3',4'-dihydroxyphenyl)-γ-valerolactone	191666-22-5	✓	reference standard	7
(4R)-5-(3',4'-Dihydroxyphenyl)-γ-valerolactone-4'-O-sulfate	x	x	4-hydroxybenzoic acid-3-sulfate	5
kaempferol	520-18-3	✓	reference standard	7
4-methoxybenzoic acid-3-O-glucuronide	synthetic	✓	reference standard	3
4-methoxybenzoic acid-3-sulfate	synthetic	✓	reference standard	1
benzoic acid-4-O-glucuronide	synthetic	✓	reference standard	2
3-methoxybenzoic acid-4-O-glucuronide	synthetic	✓	reference standard	3
3-hydroxyhippuric acid	1637-75-8	✓	reference standard	6
4-hydroxybenzoic acid 3-sulfate	x	x	3-hydroxybenzoic acid-4-Sulfate	3
3-hydroxycinnamic acid-4-O-glucuronide	1093679-71-0	✓	reference standard	1
benzoic acid-3-O-glucuronide	x	x	benzoic acid-4-O-glucuronide	4
4-hydroxyphenylproprionic acid-3-O-glucuronide	synthetic	✓	reference standard	1
3-methoxyphenylacetic acid-4-sulfate	38339-06-9	✓	reference standard	5
3-(4-hydroxyphenyl)propanoic acid-3-sulfate	1187945-70-5	✓	reference standard	5
3,5-dihydroxyphenylpropanoic acid 3-O-glucuronide	synthetic	✓	reference standard	5
methoxycinnamic acid-O-glucuronide	x	x	4-methoxycinnamic acid	6

4-methoxycinnamic acid	830-09-1	✓	reference standard	3
3-methoxycinnamic acid	6099-04-3	✓	reference standard	5
delphinidin glucoside	6906-38-3	✓	reference standard	1
cyanidin-3-galactoside	27661-36-5	✓	reference standard	1
petunidin glucoside	6988-81-4	✓	reference standard	1
peonidin-3-O-galactoside	28148-89-2	✓	reference standard	1
peonidin-3-O-glucoside	6906-39-4	✓	reference standard	1
peonidin-O-diGlucuronide	x	x	peonidin-3-O-glucoside	6
Malvidin-3-galactoside	30113-37-2	✓	reference standard	1
Kaempferol-3-O-rutinoside	17650-84-9	✓	reference standard	5
3-(4-methoxyphenyl)propanoic acid-3-O-glucuronide	1187945-72-7	x	3-(4-methoxyphenyl)propionic acid	4
3-(4-methoxyphenyl)propionic acid	1929-29-9	✓	reference standard	3
Kaempferol -7-O-glucopyranoside	16290-07-6	✓	reference standard	5
methoxyphenylacetic acid-O-glucuronide	x	x	4-methoxyphenylacetic acid	3
2-hydroxy-4-methoxybenzaldehyde	673-22-3	✓	reference standard	3
hydroxy-methoxybenzyldehyde-O-glucuronide	x	x	3-hydroxy-4-methoxybenzaldehyde	4
4-methoxyphenylacetic acid	104-01-8	✓	reference standard	3
4-hydroxyphenylacetic acid	156-38-7	✓	reference standard	3
1,3,5-trihydroxybenzene	108-73-6	✓	reference standard	3
3-hydroxy-4-methoxyphenylacetic acid	1131-94-8	✓	reference standard	5
ascorbic acid-sulfate	x	x	3,4-dihydroxybenzoic acid	6
hydroxy-methoxycinnamic acid-sulfate	x	x	3-(3-hydroxy-4-methoxyphenyl)propionic acid	4
hydroxy-methoxycinnamic acid-sulfate	x	x	3-(3-hydroxy-4-methoxyphenyl)propionic acid	6
pyridoxic acid-sulfate	x	x	3-(3-hydroxyphenyl)propionic acid	5
dihydroxy-methoxycinnamic acid-sulfate	x	x	4-hydroxycinnamic acid	6
hippuric acid-sulfate methyl ester	x	x	3,4-dihydroxybenzoic acid	6
hydroxy-dimethoxyphenylacetic acid-sulfate	x	x	3,4-dihydroxybenzoic acid	6
methoxybenzoic acid-sulfate	x	x	4-hydroxy-3-methoxybenzoic acid	5
methoxyphenylpropanoic acid-sulfate	x	x	3,4-dihydroxybenzoic acid	4
Dimethoxybenzaldehyde-sulfate	x	x	4-hydroxy-3-methoxybenzoic acid	4

hydroxy-dimethoxyphenylacetic acid-sulfate	x	x	3,4-dihydroxybenzoic acid	4
hydroxy-methoxybenzaldehyde-sulfate	x	x	4-hydroxy-3-methoxybenzoic acid	4
valeric acid-sulfate	x	x	3,4-dihydroxybenzoic acid	5
2-(hydroxyphenyl)acetic acid-4-sulfate	x	x	3,4-dihydroxybenzoic acid	4
2-(hydroxyphenyl)acetic acid-4-sulfate	x	x	3,4-dihydroxybenzoic acid	4