

Supplemental Data: Multiple Reaction Monitoring (MRM) Transitions, Declustering Potential (DP) and Collision Energy (CE) for each Microbial and Conjugate Metabolite Identified in this Study.

Analyte	MRM transitions	Identified by	DP	CE	Quantified as
Hydroxybenzoic acids					
2,4-dihydroxybenzoic acid	153/109	STD ^a	-50	-20	STD
2,6-dihydroxybenzoic acid	153/109	STD	-50	-20	STD
2,5-dihydroxybenzoic acid	153/109	STD	-50	-20	STD
3,5-dihydroxybenzoic acid	153/109	STD	-50	-20	STD
Protocatechuic acid	153/109	STD	-50	-20	STD
Vanillic acid	167/152	STD	-50	-20	STD
Syringic acid	197/121	STD	-50	-25	STD
4-hydroxybenzoic acid	137/93	STD	-50	-16	STD
3-hydroxybenzoic acid	137/93	STD	-50	-16	STD
4-hydroxyhippuric acid	194/100	STD	-50	-20	STD
3-hydroxyhippuric acid	194/150	PIS ^b	-50	-20	4-hydroxyhippuric acid
Gallic acid	169/125	STD	-40	-20	STD
4-O-methyl gallic acid	167/108	STD	-50	-26	STD
Methyl gallic acid	167/108	PIS	-50	-26	4-O-methyl gallic acid
Methyl gallic sulfate	263/183	PIS	-50	-25	Gallic acid
Ethylgallate	197/169	STD	-50	-25	Gallic acid
Ethylgallate sulfate	277/197	PIS	-50	-25	Gallic acid
Ethylgallate glucuronide 1,2	373/197	PIS	-50	-25	Epicatechin-5- <i>O</i> -glucuronide
Hydroxyphenylacetic acids					
Phenylacetic acid	135/91	STD	-30	-12	STD
3-hydroxyphenylacetic acid	151/107	STD	-50	-12	STD
2-hydroxyphenylacetic acid	151/107	STD	-50	-12	STD
3,4-dihydroxyphenylacetic acid	167/123	STD	-50	-12	STD
Homovanillic acid	181/137	STD	-40	-10	Vanillic acid
Hydroxycinnamic acids					
<i>m</i> -coumaric acid	163/119	STD	-50	-30	STD
<i>o</i> -coumaric acid	163/119	STD	-50	-30	STD
<i>p</i> -coumaric acid	163/119	STD	-50	-30	STD
Caffeic acid	179/135	STD	-50	-21	STD
Ferulic acid	193/134	STD	-50	-25	STD
Sinapic acid	223/164	STD	-50	-25	STD
Hydroxyphenylpropionic acids					
3-(4-hydroxyphenyl)propionic acid	165/121	STD	-30	-16	STD
3-(3-hydroxyphenyl)propionic acid	165/121	STD	-30	-16	STD
Dihydrocaffeic acid	181/137	STD	-40	-10	STD
Flavan-3-ols					
(Epi)catechin glucuronide 1,2,3,4	465/289	PIS	-50	-25	Epicatechin-5- <i>O</i> -glucuronide
(Epi)catechin sulfate 1,2,3	369/289	PIS	-50	-25	(Epi)Catechin
Methyl (epi)catechin glucuronide 1,2,3	479/303	PIS	-50	-30	Epicatechin-5- <i>O</i> -glucuronide

Methyl (epi)catechin sulfate 1,2,3	383/303	PIS	-50	-25	(Epi)Catechin
Glycinates					
Vanilloylglycine	224/180	PIS	-50	-25	4-hydroxyhippuric acid
Feruloylglycine	250/100	PIS	-50	-25	4-hydroxyhippuric acid
Hydroxyphenylvalerolactones					
DHPV 1	207/163	PIS	-50	-25	(Epi)Catechin
DHPV 2	207/163	PIS	-50	-25	(Epi)Catechin
DHPV glucuronide 1,2	383/207	PIS	-50	-25	Epicatechin-5- <i>O</i> - glucuronide
DHPV sulfate 1,2	287/207	PIS	-50	-25	(Epi)Catechin
MHPV 1	221/162	PIS	-50	-25	(Epi)Catechin
MHPV glucuronide 1	397/221	PIS	-50	-25	Epicatechin-5- <i>O</i> - glucuronide
MHPV sulfate 1,2	301/221	PIS	-50	-25	(Epi)Catechin
Other polyphenols					
Enterolactone	297/253	STD	-50	-25	STD
Pyrogallol	125/69	STD	-50	-25	STD

^aSTD, Standard available; ^bPIS, Product Ion Scan.