

SUPPLEMENTARY MATERIAL

Metabolomic profiling of urinary phenolic compounds in postmenopausal women after consumption of dark chocolate, green tea, and fruit juice

Lorena Sánchez-Martínez^{a,b}, Nicole Tosi^c, Nicola Luigi Bragazzi^c, Letizia Bresciani^c, Daniele Del Rio^{c,d}, María Jesús Periago^{*a,b}, Pedro Mena^{+c,d}, Rocío González-Barrio^{*a,b}

^a Department of Food Technology, Food Science and Nutrition, University of Murcia. Campus Mare Nostrum, Campus de Espinardo, 30100 Murcia, Spain. E-mail: rgbbarrio@um.es, mjperi@um.es; Tel: +34 868889641

^b Biomedical Research Institute of Murcia Pascual Parrilla-IMIB, 30120 Murcia, Spain.

^c Department of Food and Drugs, University of Parma, Parma, Italy.

^d Microbiome Research Hub, University of Parma, Parma, Italy.

+Co-last author

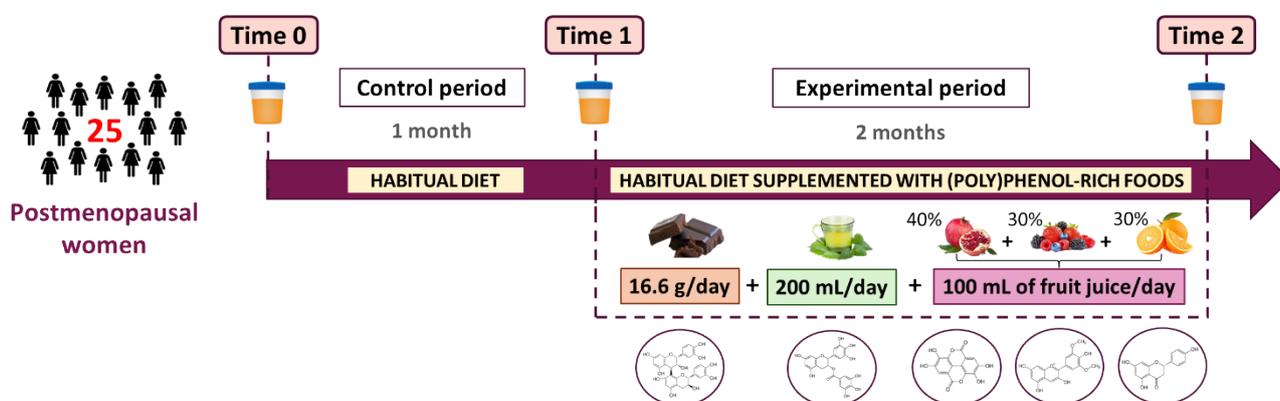


Figure S1. Dietary intervention trial design

Table S.1. Chromatographic and spectrometric properties of the monitored phenolic metabolites.

Compound detected and quantified in urine samples	RT (min)	Parent ion [M-H] ⁻ (m/z)	S-Lens	Quantifier		Qualifier(s)		STD (in bold the reference compounds used to quantify the corresponding metabolite or its coeluting isomers)	Ref.
				Product ion (m/z)	CE (V)	Product ion (m/z)	CE (V)		
Methoxy-(epi)gallocatechin-glucuronide (MeO-EGC-Glc)	4.18	495	98	319	27	175	18	4'-Methoxycinnamic acid-3'-glucuronide	1,2
(-)-Epicatechin (EC)	4.35	289	103	245	18	205,124,151	21,30,30	(-)-Epicatechin	
(Epi)catechin-glucuronide isomer 1 (EC-Glc-iso1)	4.34	465	98	289	27	113	19	4'-Hydroxycinnamic acid-3'-glucuronide	3-6
(Epi)catechin-glucuronide isomer 2 (EC-Glc-iso2)	4.93	465	98	289	27	113	19	4'-Hydroxycinnamic acid-3'-glucuronide	3-6
(Epi)catechin-sulfate (EC-S)	5.30	369	93	289	20	245	16	4'-Hydroxyphenylpropanoic acid-3'-sulfate	3-6
Myricetin-glucuronide (Myricetin-Glc)	4.70	493	90	317	27	113	30	Hesperetin-7-glucuronide	
Quercetin-3-glucuronide (Quercetin-3-Glc)	5.07	477	91	301	28	113	30	Quercetin-3-glucuronide	
Kaempferol- glucuronide (Kaempferol-Glc)	6.50	461	90	285	27	113	30	Quercetin-3-glucuronide	
Myricetin-sulfate (Myricetin-S)	6.80	397	90	317	20	179	30	Quercetin-3-sulfate	
Quercetin-3-sulfate (Quercetin-3-S)	7.60	381	84	301	24	151,179	24,24	Quercetin-3-sulfate	
Kaempferol-sulfate (Kaempferol-S)	8.00	365	90	285	20	257	30	Quercetin-3-sulfate	
Apigenin-glucuronide (Apigenin-Glc)	5.50	445	93	269	20	113,225	30,30	Naringenin-7-glucuronide	
Hesperetin-7-glucuronide (Hesperetin-Glc)	5.38	477	91	301	28	113	30	Hesperetin-7-glucuronide	
Naringenin-7-glucuronide (Naringenin-Glc)	5.25	447	84	271	25	113	30	Naringenin-7-glucuronide	
Hesperetin-sulfate (Hesperetin-S)	7.60	381	84	301	24	286	35	Quercetin-3-sulfate	
Naringenin-sulfate (Naringenin-S)	8.50	351	84	271	25	151,231	39,25	Quercetin-3-sulfate	
5-(3',4',5'-Trihydroxyphenyl)-γ-valerolactone (3',4',5'-TriHPVL)	2.49	223	75	179	21	138	26	5-(3',4',5'-Trihydroxyphenyl)-γ-valerolactone	
5-(Dihydroxyphenyl)-γ-valerolactone-glucuronide (3',4',5') isomer 1 (DiHPVL-Glc-iso1)	3.29	399	87	223	30	113	25	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide	1,7,8
5-(Dihydroxyphenyl)-γ-valerolactone-glucuronide (3',4',5') isomer 2 (DiHPVL-Glc-iso2)	4.30	399	87	223	30	113	25	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide	3-6
5-(Dihydroxyphenyl)-γ-valerolactone-sulfate (3',4',5' isomers) (DiHPVL-S)	5.33	303	84	223	20	179	30	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-sulfate	1,7
5-(Hydroxyphenyl)-γ-valerolactone-methoxy-glucuronide (3',4',5') isomer 1 (HPVL-MeO-Glc-iso1)	4.50	413	87	222	30	222,113	30,30	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide	1,7
5-(Hydroxyphenyl)-γ-valerolactone-methoxy-glucuronide (3',4',5') isomer 2 (HPVL-MeO-Glc- iso2)	3.70	413	87	222	30	237,113	30,30	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide	1,7
5-(Hydroxyphenyl)-γ-valerolactone-methoxy-sulfate (3',4',5') isomer 1 (HPVL-MeO-S-iso1)	5.56	317	97	237	23	222	40	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-sulfate	
5-(3',5'-Dihydroxyphenyl)-γ-valerolactone (3',5'-DiHPVL)	3.98	207	72	122	21	163,121,119	18,22,21	5-(3',5'-Dihydroxyphenyl)-γ-valerolactone	
5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide (5'-HPVL-3'-Glc)	3.07	383	92	207	27	113	30	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide	
5-(5'Hydroxyphenyl)-γ-valerolactone-3'sulfate (5'-HPVL-3'-S)	5.05	287	96	207	23	163	35	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-sulfate	
5-(3',4'-Dihydroxyphenyl)-γ-valerolactone (3',4'-DiHPVL)	4.30	207	72	163	18	121,122,123	22,21,20	5-(3',4'-Dihydroxyphenyl)-γ-valerolactone	
5-(3'-Hydroxyphenyl)-γ-valerolactone-4'-glucuronide (3'-HPVL-4'-Glc)	4.13	383	92	207	27	113	30	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide	7
5-(4'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide (4'-HPVL-3'-Glc)	4.38	383	92	207	27	113	30	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide	
5-(Hydroxyphenyl)-γ-valerolactone-sulfate (HPVL-S) (3',4'isomers)	5.70	287	96	207	23	163	35	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-sulfate	
5-Phenyl-γ-valerolactone-methoxy-glucuronide (3',4') isomer 1 (PVL-MeO-Glc-iso1)	4.55	397	90	221	30	113	30	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide	7,9,10

5-Phenyl-γ-valerolactone-methoxy-glucuronide (3',4') isomer 2 (PVL-MeO-Glc-iso2)	5.05	397	90	221	30	113	30	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide	7,9,10
5-Phenyl-γ-valerolactone-methoxy-sulfate (3',4') isomer 1 (PVL-MeO-S-iso1)	5.67	301	87	221	23	206	40	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-sulfate	3,7,9,10
5-Phenyl-γ-valerolactone-methoxy-sulfate (3',4') isomer 2 (PVL-MeO-S-iso2)	5.90	301	87	221	23	206	40	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-sulfate	3,7,9-11
5-(3'-Hydroxyphenyl)-γ-valerolactone (3'-HPVL)	5.04	191	67	106	31	147,107	16,24	5-(3'-Hydroxyphenyl)-γ-valerolactone	
5-Phenyl-γ-valerolactone-4'-glucuronide (PVL-4'-Glc)	4.26	367	93	191	25	113	19	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide	7,8,10
5-Phenyl-γ-valerolactone-3'-glucuronide (PVL-3'-Glc)	4.49	367	93	191	25	113	19	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide	5,7-10,12
5-Phenyl-γ-valerolactone-4'-sulfate (PVL-S-4')	5.49	271	93	191	23	147,106	35,48	5-(Phenyl)-γ-valerolactone-3'-sulfate	
5-Phenyl-γ-valerolactone-3'-sulfate (PVL-S-3')	5.85	271	93	191	23	147,106	35,48	5-(Phenyl)-γ-valerolactone-3'-sulfate	
5-Phenyl-γ-valerolactone-sulfate-glucuronide (3',4' isomers) (PVL-S-Glc)	4.85	463	87	287	27	207,383,113	40,20,19	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide	5,7,9,10
4-Hydroxy-5-(3',4'-dihydroxyphenyl)valeric acid (4-OH-3',4'-DiHPVA)	2.80	225	83	101	20	181,179	23,20	5-(3',4'-Dihydroxyphenyl)-γ-valerolactone	7,8,13
4-Hydroxy-5-(hydroxyphenyl)valeric acid-sulfate (3',4' isomers) (4-OH-HPVA-S)	4.83	305	95	225	20	207,181	30,20	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-sulfate	7
4-Hydroxy-5-(phenyl)valeric acid-glucuronide (3'/4' isomers) (4-OH-PVA-Glc)	4.35	385	95	113	30	209	30	5-(5'-Hydroxyphenyl)-γ-valerolactone-3'-glucuronide	8,13,14
3',4'-Dihydroxycinnamic acid (3',4'-DiHCA)	3.80	179	62	135	19			3',4'-Dihydroxycinnamic acid	
3'-Hydroxycinnamic acid-4'-glucuronide (3'-HCA-4'-Glc)	2.70	355	98	179	21	113	18	3'-Hydroxycinnamic acid-4'-glucuronide	
4'-Hydroxycinnamic acid-3'-glucuronide (4'-HCA-3'-Glc)	4.12	355	98	179	21	113	18	4'-Hydroxycinnamic acid-3'-glucuronide	
3'-Hydroxycinnamic acid-4'-sulfate (3'-HCA-4'-S)	4.80	259	62	179	20	135	25	3-(4'-Hydroxyphenyl)propanoic acid-3'-sulfate	8
4'-Hydroxycinnamic acid-3'-sulfate (4'-HCA-3'-S)	5.20	259	62	179	20	135	25	3-(4'-Hydroxyphenyl)propanoic acid-3'-sulfate	4,15
4'-Hydroxy-3'-methoxycinnamic acid (3'-MeO-4'-HCA)	4.83	193	71	134	19	178	18	4'-Hydroxy-3'-methoxycinnamic acid	
3'-Methoxycinnamic acid-4'-glucuronide (3'-MeO-CA-4'-Glc)	3.88	369	93	193	20	113,134,178	18,39,32	3'-Methoxycinnamic acid-4'-glucuronide	
4'-Methoxycinnamic acid-3'-glucuronide (4'-MeO-CA-3'-Glc)	4.49	369	93	113	18	178,193,134	32,20,39	4'-Methoxycinnamic acid-3'-glucuronide	
3'-Methoxycinnamic acid-4'-sulfate (3'-MeO-CA-4'-S)	5.20	273	92	193	18	178,134,149	28,33,30	3'-Methoxycinnamic acid-4'-sulfate	
4'-Methoxycinnamic acid-3'-sulfate (4'-MeO-CA-3'-S)	5.45	273	92	193	18	178,134,149	28,33,30	4'-Methoxycinnamic acid-3'-sulfate	
N-(4'-Hydroxy-3'-methoxy-cinnamoyl)glycine (3'-MeO-4'-HCA-Gly)	4.51	250	79	206	14	134,163	22,19	N-(4'-Hydroxy-3'-methoxy-cinnamoyl)glycine	
2'-Hydroxycinnamic acid (2'-HCA)	5.10	163	62	119	19	93	38	3'-Hydroxycinnamic acid	16
3'-Hydroxycinnamic acid (3'-HCA)	4.89	163	62	119	19	93	38	3'-Hydroxycinnamic acid	
4'-Hydroxycinnamic acid (4'-HCA)	4.65	163	62	119	19	93	38	3'-Hydroxycinnamic acid	16
Cinnamic acid-4'-glucuronide (CA-4'-Glc)	4.40	339	90	163	20	113	16	3-(4'-Hydroxyphenyl)propanoic acid-3'-glucuronide	17
Cinnamic acid-3'-glucuronide (CA-3'-Glc)	4.60	339	90	163	20	113	16	3-(4'-Hydroxyphenyl)propanoic acid-3'-glucuronide	8
Cinnamic acid-4'-sulfate (CA-4'-S)	5.21	243	62	163	20	119	35	3-(4'-Hydroxyphenyl)propanoic acid-3'-sulfate	4,17
Cinnamic acid-3'-sulfate (CA-3'-S)	5.47	243	62	163	20	119	35	3-(4'-Hydroxyphenyl)propanoic acid-3'-sulfate	8
3-(3',4'-Dihydroxyphenyl)propanoic acid (3',4'-DiHPPA)	3.18	181	64	137	14	119,121	13,10	3-(3',4'-Dihydroxyphenyl)propanoic acid	
3-(3'-Hydroxyphenyl)propanoic acid-4'-glucuronide (3'-HPPA-4'-Glc)	3.85	357	63	181	21	113	22	3-(4'-Hydroxyphenyl)propanoic acid-3'-glucuronide	8
3-(4'-Hydroxyphenyl)propanoic acid-3'-glucuronide (4'-HPPA-3'-Glc)	9.90	357	63	181	21	113	22	3-(4'-Hydroxyphenyl)propanoic acid-3'-	

3-(4'-Hydroxyphenyl)propanoic acid-sulfate (4'-HPPA-3'-S)	5.00	261	96	181	20	137	25	glucuronide
3-(4'-Hydroxy-3'-methoxyphenyl)propanoic acid (3'-MeO-4'-HPPA)	4.63	195	73	136	21	151,165	22,18	3-(4'-Hydroxyphenyl)propanoic acid-3'-sulfate
3-(3'-Hydroxy-4'-methoxyphenyl)propanoic acid (4'-MeO-3'-HPPA)	4.80	195	73	136	21	151	22	3-(4'-Hydroxy-3'-methoxyphenyl)propanoic acid
3-(3'-Methoxyphenyl)propanoic acid-4'-glucuronide (3'-MeO-PPA-4'-Glc)	4.08	371	90	195	26	113	21	3-(4'-Methoxy-phenyl)propanoic acid-3'-glucuronide
3-(4'-Methoxyphenyl)propanoic acid-3'-glucuronide (4'-MeO-PPA-3'-Glc)	4.52	371	90	195	26	113	21	3-(4'-Methoxy-phenyl)propanoic acid-3'-glucuronide
3-(3'-Methoxyphenyl)propanoic acid-4'-sulfate (3'-MeO-PPA-4'-S)	5.05	275	75	195	31	136	17	3-(3'-Methoxy-phenyl)propanoic acid-4'-sulfate
3-(4'-Methoxyphenyl)propanoic acid-3'-sulfate (4'-MeO-PPA-3'-S)	5.35	275	75	195	31	136	17	3-(3'-Methoxy-phenyl)propanoic acid-4'-sulfate
3-(3'-Hydroxyphenyl)propanoic acid (3'-HPPA)	4.59	165	48	121	15	119	20	3-(3'-Hydroxyphenyl)propanoic acid
3-(Phenyl)propanoic acid-4'-glucuronide (PPA-4'-Glc)	4.13	341	90	165	20	113	18	3-(4'-Hydroxyphenyl)propanoic acid-3'-glucuronide
3-(Phenyl)propanoic acid-3'-glucuronide (PPA-3'-Glc)	4.40	341	90	113	18	165	20	3-(4'-Hydroxyphenyl)propanoic acid-3'-glucuronide
3-(Phenyl)propanoic acid-sulfate (3',4' isomers) (PPA-S)	5.30	245	90	165	20	121	15	3-(4'-Hydroxyphenyl)propanoic acid-3'-sulfate
4'-Hydroxy-3'-methoxyphenylacetic acid (3'-MeO-4'-HPAA)	3.93	181	64	137	14	121,122,119,166	10,30,13,30	4'-Hydroxy-3'-methoxy-phenylacetic acid
3'-Hydroxy-4'-methoxyphenylacetic acid (4'-MeO-3'-HPAA)	4.10	181	64	137	14	121,122,119,166	10,30,13,30	3-Methoxypropanoic acid-4-sulfate
3'-Methoxy-phenylacetic acid-4'-sulfate (3'-MeO-PAA-4'-S)	4.40	261	96	137	25	181	20	3-Methoxypropanoic acid-4-sulfate
4'-Methoxy-phenylacetic acid-3'-sulfate (4'-MeO-PAA-3'-S)	4.60	261	96	137	25	181	20	3-Methoxypropanoic acid-4-sulfate
3'-Hydroxyphenylacetic acid (3'-HPAA)	3.75	151	40	107	10	136	17	3'-Hydroxyphenylacetic acid
4'-Hydroxyphenylacetic acid (4'-HPAA)	2.99	151	40	107	10	136	17	3'-Hydroxyphenylacetic acid
3,4,5-Trihydroxybenzoic acid (3,4,5-TriHBA)	1.00	169	68	125	20			3,4,5-Trihydroxybenzoic acid
4-Methoxy-3,5-Dihydroxybenzoic acid (4-MeO-3,5-DiHBA)	2.20	183	70	168	26	139	20	3-Methoxy-4,5-Dihydroxybenzoic acid
4-Hydroxy-3,5-Dimethoxybenzoic acid(3,5-DiMeO-4-HBA)	4.15	197	70	182	20	153	14	3,4,5-Trihydroxybenzoic acid
Hydroxy-methoxybenzoic acid-sulfate (MeO-HBA-S)	4.30	263	68	183	20	168	26	3-Methoxybenzoic acid-4-sulfate
3,4-Dihydroxybenzoic acid (3,4-DiHBA)	1.45	153	64	109	20	108	27	3,4-Dihydroxybenzoic acid
3-Hydroxybenzoic acid-4-glucuronide (3-HBA-4-Glc)	1.24	329	81	153	21	113	18	3-Hydroxybenzoic acid-4-glucuronide
4-Hydroxybenzoic acid-3-glucuronide (4-HBA-3-Glc)	1.92	329	81	153	21	113	18	4-Hydroxybenzoic acid-3-glucuronide
Hydroxybenzoic acid-sulfate (3,4 isomers) (HBA-S)	4.10	233	85	153	20	109	33	4-Hydroxybenzoic acid-3-sulfate
4-Hydroxy-3-methoxybenzoic acid (3-MeO-4-HBA)	2.88	167	60	152	18	108,123	21,17	4-Hydroxy-3-methoxybenzoic acid
3-Methoxybenzoic acid-4-glucuronide (3-MeO-BA-4-Glc)	1.68	343	92	167	23	152,113	40,17	3-Methoxybenzoic acid-4-glucuronide
4-Methoxybenzoic acid-3-glucuronide (4-MeO-BA-3-Glc)	3.70	343	92	113	17	167,152	23,40	4-Methoxybenzoic acid-3-glucuronide
3-Methoxybenzoic acid-4-sulfate (3'-MeO-BA-4-S)	4.47	247	72	167	17	152,123	27,17	3-Methoxybenzoic acid-4-sulfate
4-Methoxybenzoic acid-3-sulfate (4'-MeO-BA-3-S)	4.75	247	72	167	17	152,123	27,17	3-Methoxybenzoic acid-4-sulfate
4-Hydroxybenzoic acid (4-HBA)	2.60	137	70	93	16	92	26	4-Hydroxybenzoic acid
Benzoic acid-4-glucuronide (BA-4-Glc)	1.26	313	78	113	15	137	20	Benzoic acid-4-glucuronide
Benzoic acid-3-glucuronide (BA-3-Glc)	1.79	313	78	113	15	137	20	Benzoic acid-4-glucuronide
Benzoic acid-4-sulfate (BA-4-S)	4.20	217	70	137	20	93	16	Benzoic acid-4-sulfate
Benzoic acid-3-sulfate (BA-3-S)	4.63	217	70	137	20	93	16	Benzoic acid-4-sulfate
1,2,3-Trihydroxybenzene (1,2,3-TriOH-Benz)	1.08	125	68	97	15	81	20	1,2,3-Trihydroxybenzene
2-Hydroxy-3/6-methoxybenzene-1-sulfate or 3-Hydroxy-2-methoxybenzene-1-sulfate (MeO-Pyr-S)	4.70	219	68	124	24	139	20	3-Methoxybenzoic acid-4-sulfate

1,2-Dihydroxybenzene (1,2-DiOH-Benz)	2.10	109	68	108	20	81	20	1,2-Dihydroxybenzene	
2-Hydroxy-benzene-1-glucuronide (Cat-Glc)	2.70	285	78	109	27	113	15	Benzoic acid-4-glucuronide	8
2-Hydroxy-benzene-1-sulfate (Cat-S)	4.55	189	70	109	20	81	20	Benzoic acid-4-sulfate	3,4,8,16
2-Hydroxy-4/5-methylbenzene-1-sulfate (Met-Cat-S)	5.22	203	70	123	20	108	26	3-Methoxybenzoic acid-4-sulfate	
4-Hydroxybenzaldehyde (4-HBAL)	3.60	121	89	92	27	91	22	4-Hydroxybenzaldehyde	
Dimethylellagic acid-glucuronide (DMEA-Glc)	5.10	505	91	329	28	113	30	Urolithin A-8-glucuronide	
3,8,9-Trihydroxy-urolithin (Uro-C)	5.05	243	122	187	32	171,199	29,29	Urolithin C	
3,8-Dihydroxy-urolithin and/or 3,9-Dihydroxy-urolithin ((ISO)Uro-A)	5.49	227	92	198	36	171,181,183	29,30,24	Urolithin A	
3-Hydroxy-urolithin-8-glucuronide and/or 3-Hydroxy-urolithin-9-glucuronide ((ISO)Uro-A-Glc)	4.89	403	78	227	37	113	15	Urolithin A-8-glucuronide	
3-Hydroxy-urolithin-8-sulfate and/or 3-Hydroxy-urolithin-9-sulfate ((ISO)Uro-A-S)	6.60	307	78	227	19			Urolithin A-8-sulfate	
3-Hydroxy-urolithin (Uro-B)	6.15	211	116	167	27	139,117	34,36	Urolithin B	
Urolithin-3-glucuronide (Uro-B-Glc)	5.40	387	84	211	30	113	30	Urolithin B-3-glucuronide	
Urolithin-3-sulfate (Uro-B-S)	8.00	291	86	211	19			Urolithin A-8-sulfate	
4-Hydroxyhippuric acid (4-HHA)	1.66	194	72	100	11	150	15	4-Hydroxyhippuric acid	
Hippuric acid (HA)	3.20	178	61	134	15	77.2	22	Hippuric acid	

RT: retention time; CE: collision energy; STD: standard use for quantification; Ref.: reference in the literature used for identification of compounds without an available standard. Nomenclature of metabolites is reported as proposed by Kay et al.¹⁹, as well as Curti et al.²⁰ and the abbreviations are reported under brackets.

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