

Table S1 Supplementary Information. Optimized SRM conditions used for quantification for the analysis of phenolic compounds by UPLC-MS/MS.

Phenolic compound	MW	Quantification			Standard used for quantification
		SRM	Cone voltage (v)	Collision energy (eV)	
Catechol	110	108.9 > 90.9	40	15	Catechol
Catechol sulfate	190	189 > 109	20	15	Catechol
Catechol glucuronide	286	285 > 123	40	15	Catechol
Pyrogallol sulfate	206	205 > 125	20	15	Catechol
Methyl pyrogallol sulfate	220	219 > 124	20	25	Catechol
Pyrogallol glucuronide	302	301 > 125	20	10	Catechol
Pyrogallol glucuronide-sulfate	382	381 > 125	20	10	Catechol
<i>p</i> -Hydroxybenzoic acid	138	137 > 93	30	15	<i>p</i> -Hydroxybenzoic acid
Hydroxybenzoic acid	138	137 > 93	30	15	<i>p</i> -Hydroxybenzoic acid
Protocatechuic acid	154	153 > 109	40	15	Protocatechuic acid
Gallic acid	170	169 > 125	35	10	Gallic acid
Gallic acid hexoside	332	331 > 169	40	15	Gallic acid
Mono- <i>O</i> -galloylquinic acid	344	343 > 191	40	15	Gallic acid
Di- <i>O</i> -galloylquinic acid	496	495 > 191	40	25	Gallic acid
Tri- <i>O</i> -galloylquinic acid	648	647 > 495	40	15	Gallic acid
Tetra- <i>O</i> -galloylquinic acid	630	629 > 477	40	15	Gallic acid
Mono- <i>O</i> -galloylshikimic acid	326	325 > 169	40	20	Gallic acid
Di- <i>O</i> -galloylshikimic acid	478	477 > 325	40	20	Gallic acid
Gallic acid sulphate	250	249 > 169	35	15	Gallic acid
Gallic acid glucuronide	346	345 > 169	35	15	Gallic acid
Syringic acid	198	197 > 182	30	10	Syringic acid
Ellagic acid arabinoside	434	433 > 300	40	30	Ellagic acid
Ellagic acid glucuronide	478	477 > 301	40	20	Ellagic acid
Strictinin ellagitannin	634	633 > 301	40	30	Ellagic acid
<i>p</i> -Hydroxyphenylacetic acid	152	151 > 107	20	10	<i>p</i> -Hydroxyphenylacetic acid
Dihydroxyphenylacetic acid	168	167 > 123	20	10	3,4-Dihydroxyphenylacetic acid

3-(4-Hydroxyphenyl)propionic acid	166	165 > 121	20	10	3-(4-Hydroxyphenyl)propionic acid
Hydroxyphenylpropionic acid	166	165 > 121	20	10	3-(4-Hydroxyphenyl)propionic acid
3-(2',4'-Dihydroxyphenyl)propionic acid	181	181 > 137	20	15	3-(2',4'-Dihydroxyphenyl)propionic acid
Dihydroxyphenylpropionic acid	181	181 > 137	20	15	3-(2',4'-Dihydroxyphenyl)propionic acid
Hippuric acid	179	178 > 134	40	10	Hippuric acid
Catechin	290	289 > 245	45	15	Catechin
Gallocatechin – catechin	594	593 > 289	40	30	Catechin
Catechin sulfate	370	369 > 289	40	20	Catechin
Catechin glucuronide	466	465 > 289	40	20	Catechin
Methyl catechin glucuronide	480	479 > 303	40	25	Catechin
Epicatechin	290	289 > 245	45	15	Epicatechin
Epigallocatechin	306	305 > 125	40	15	Epicatechin
Epicatechin gallate	442	441 > 169	40	20	Epicatechin
Epigallocatechin gallate	458	457 > 169	40	15	Epicatechin
Methyl epicatechin sulfate	384	383 > 303	45	15	Epicatechin
Methyl epicatechin glucuronide	480	479 > 303	40	25	Epicatechin
Dimer	578	577 > 289	45	20	Dimer B ₂
Trimer	865	865 > 287	60	30	Dimer B ₂
Quercetin-3- <i>O</i> -glucoside	464	463 > 301	45	25	Quercetin
Quercetin glucoside	464	463 > 301	45	25	Quercetin
Quercetin arabinoside	434	433 > 300	45	20	Quercetin
Quercetin rhamnoside	448	447 > 301	40	15	Quercetin
Dihydroquercetin	304	303 > 285	45	15	Quercetin
Quercetin galloyl hexoside	616	615 > 463	40	30	Quercetin
Kaempferol-3- <i>O</i> -glucoside	448	447 > 285	45	15	Kaempferol
Kaempferol-3- <i>O</i> -rhamnoside	432	431 > 285	45	20	Kaempferol
Kaempferol-3- <i>O</i> -rutinoside	594	593 > 285	50	25	Kaempferol
Dihydrokaempferol	288	287 > 259	45	10	Kaempferol
Dihydrokaempferol hexoside	450	449 > 269	40	15	Kaempferol
Myricetin glucoside	480	479 > 317	45	20	Myricetin
Myricetin rhamnoside	464	463 > 317	50	25	Myricetin
Cyanidin-3- <i>O</i> -glucoside *	450	449 > 287	40	20	Cyanidin-3- <i>O</i> -Glucoside
Cyanidin arabinoside *	420	419 > 287	40	20	Cyanidin-3- <i>O</i> -Glucoside
Delphinidin arabinoside *	436	435 > 303	40	20	Cyanidin-3- <i>O</i> -Glucoside
Delphinidin glucoside *	466	465 > 303	40	20	Cyanidin-3- <i>O</i> -Glucoside

Pelargonidin arabinoside *	404	403 > 271	40	20	Cyanidin-3- <i>O</i> -Glucoside
Pelargonidin glucoside *	434	433 > 271	40	20	Cyanidin-3- <i>O</i> -Glucoside
Peonidin arabinoside *	434	433 > 301	40	20	Cyanidin-3- <i>O</i> -Glucoside
Peonidin glucoside *	464	463 > 301	40	20	Cyanidin-3- <i>O</i> -Glucoside
Hydroxy urolithin (urolithin B) *	212	213 > 141	40	20	Hydroxy urolithin (urolithin B)
Dihydroxy urolithin (urolithin A) *	230	229 > 157	40	20	Dihydroxy urolithin (urolithin A)
Trihydroxy urolithin (urolithin C) *	246	245 > 155	40	30	Trihydroxy urolithin (urolithin C)
Hydroxy urolithin glucuronide	388	387 > 211	40	20	Hydroxy urolithin (urolithin B)
Dihydroxy urolithin glucuronide	404	403 > 227	40	30	Dihydroxy urolithin (urolithin A)
Tetrahydroxy urolithin *	262	261 > 171	40	25	Trihydroxy urolithin (urolithin C)
Tetrahydroxy urolithin sulfate	340	339 > 259	40	20	Trihydroxy urolithin (urolithin C)
Pentahydroxy urolithin *	278	277 > 187	40	30	Trihydroxy urolithin (urolithin C)

MW: molecular weight (g/mol)

* ESI positive