

Supplementary data

Table 1S. Optimized SRM conditions used for quantification and identification for the analysis of ferulic acid-derived phenolic compounds and their generated metabolites, and the standard compound used for its quantification or tentative quantification by UPLC–MS/MS.

Phenolic compound	Quantification			Identification			MS ² fragments	Standard used for its (tentative) quantification
	SRM	Cone voltage (V)	Collision energy (eV)	SRM	Cone voltage (V)	Collision energy (eV)		
Catechol	108.9>90.9	40	15	-	-	-	90.9	Catechol
Methyl catechol	123>109	40	15	-	-	-	109	Catechol
Catechol sulphate	189>109	40	15	-	-	-	109	Catechol
Catechol glucuronide	285>109	40	15	-	-	-	109	Catechol
Methyl catechol sulphate	203>123	40	15	203>109	40	20	123, 109	Catechol
Methyl catechol glucuronide	299>123	40	15	299>109	40	20	123, 109	Catechol
Hydroxybenzoic acid	137>93	30	15	-	-	-	93	<i>p</i> -Hydroxybenzoic acid
Hydroxybenzoic acid sulphate	217>137	35	15	217>93	35	20	137, 93	<i>p</i> -Hydroxybenzoic acid
Hydroxybenzoic acid glucuronide	313>137	35	15	313>93	35	20	137, 93	<i>p</i> -Hydroxybenzoic acid
Protocatechuic acid	153>109	40	15	-	-	-	109	Protocatechuic acid
Protocatechuic acid sulphate	233>153	40	15	233>109	40	20	153, 109	Protocatechuic acid
Protocatechuic acid glucuronide	329>153	40	20	329>109	40	25	153, 109	Protocatechuic acid
Hydroxytyrosol	153>123	35	15	153>95	35	25	123, 95	Hydroxytyrosol
Hydroxytyrosol sulphate	233>153	35	15	233>123	35	20	153, 123	Hydroxytyrosol
Hydroxytyrosol glucuronide	329>153	35	15	329>123	35	20	153, 123	Hydroxytyrosol
Phenylacetic acid	135>91	20	5	-	-	-	91	Phenylacetic acid
<i>p</i> -Hydroxyphenylacetic acid	151>107	20	10	-	-	-	107	<i>p</i> -Hydroxyphenylacetic acid
<i>m</i> -Hydroxyphenylacetic acid	151>107	20	10	-	-	-	107	<i>p</i> -Hydroxyphenylacetic acid
<i>o</i> -Hydroxyphenylacetic acid	151>107	20	10	-	-	-	107	<i>p</i> -Hydroxyphenylacetic acid
Hydroxyphenylacetic acid sulphate	231>151	40	15	231>107	40	20	151, 107	<i>p</i> -Hydroxyphenylacetic acid
Hydroxyphenylacetic acid glucuronide	327>151	40	15	327>107	40	20	151, 107	<i>p</i> -Hydroxyphenylacetic acid
Dihydroxyphenylacetic acid	167>123	20	10	167>108	20	20	123, 108	3,4-Dihydroxyphenylacetic acid
Dihydroxyphenylacetic acid sulphate	247>167	35	15	247>123	35	25	167, 123, 108	3,4-Dihydroxyphenylacetic acid
Dihydroxyphenylacetic acid glucuronide	343>167	40	25	343>123	40	30	167, 123, 108	3,4-Dihydroxyphenylacetic acid
Phenylpropionic acid	149>105	20	5	-	-	-	105	3-(4-Hydroxyphenyl)propionic acid
Hydroxyphenylpropionic acid	165>121	20	10	-	-	-	121	3-(4-Hydroxyphenyl)propionic acid
Hydroxyphenylpropionic acid sulphate	245>165	35	15	245>121	35	20	165, 121	3-(4-Hydroxyphenyl)propionic acid
Hydroxyphenylpropionic acid glucuronide	341>165	40	25	341>121	40	30	165, 121	3-(4-Hydroxyphenyl)propionic acid
Dihydroxyphenylpropionic acid	181>137	20	15	-	-	-	137	3-(2,4-Dihydroxyphenyl)propionic acid
Dihydroxyphenylpropionic acid sulphate	261>181	40	15	261>137	40	25	181, 137, 109	3-(2,4-Dihydroxyphenyl)propionic acid
Dihydroxyphenylpropionic acid glucuronide	357>181	40	10	357>137	40	20	181, 137, 109	3-(2,4-Dihydroxyphenyl)propionic acid
Vanillic acid	167>123	30	10	167>152	30	15	152, 123	Vanillic acid
Vanillic acid sulphate	247>167	40	10	247>123	40	15	167, 152, 123	Vanillic acid
Vanillic acid glucuronide	343>167	40	10	343>123	40	15	167, 152, 123	Vanillic acid
Homovanillic acid	181>137	25	10	181>122	25	20	137, 122, 105	Vanillic acid
Homovanillic acid sulphate	261>181	40	15	261>137	40	25	181, 137, 122, 105	Vanillic acid
Homovanillic acid glucuronide	357>181	40	20	357>137	40	25	181, 137, 122, 105	Vanillic acid
Caffeic acid	179>135	35	10	179>117	35	15	135, 117	Caffeic acid

Caffeic acid sulphate	259>179	35	15	259>135	35	20	179, 135	Caffeic acid
Caffeic acid glucuronide	355>179	40	15	355>135	40	20	179, 135	Caffeic acid
Coumaric acid	163>119	35	10	163>93	35	20	119, 93	<i>p</i> -Coumaric acid
Coumaric acid sulphate	243>163	35	15	243>119	35	20	163, 119	<i>p</i> -Coumaric acid
Coumaric acid glucuronide	339>163	35	15	339>119	35	20	163, 119	<i>p</i> -Coumaric acid
Ferulic acid	193>134	30	15	193>178	30	20	178, 134	Ferulic acid
Ferulic acid sulphate	273>193	35	15	273>134	35	20	193, 178, 149, 134	Ferulic acid
Ferulic acid glucuronide	369>193	35	15	369>134	35	20	193, 178, 149, 134	Ferulic acid
Dihydroferulic acid	195>136	35	10	195>151	35	15	177, 151, 136, 123	Ferulic acid
Dihydroferulic acid sulphate	275>195	35	15	275>136	35	20	195, 151, 136	Ferulic acid
Dihydroferulic acid glucuronide	371>195	35	20	371>136	35	25	195, 151, 136	Ferulic acid
Huppuric acid	178>134	40	10	178>77	40	20	134, 77	Caffeic acid
Hydroxyhippuric acid	194>100	40	10	194>93	40	15	100, 93	Caffeic acid

MS² fragments: MS² daughter ions produced from [M-H]⁻ fragmentation