

Supporting Information Table 1. List of target compounds analyzed by the HPLC-LTQ-Orbitrap FTMS platform (negative electrospray ionization mode) and detected in human plasma. Columns represent: A: compound name; B: elemental formula; C: molecular ion [M-H]⁻; D: LC-retention time (minutes); E: Annotation level according to the Metabolomics Society Initiative.

Metabolite name	Elemental formula	[M-H] ⁻	RT (min)	Observed fragment ions	Annotation level ^s
Phloroglucinol (1,3,5-triOH-benzene)	C6H6O3	125.0244	5.11		1
Gallic acid	C7H6O5	169.0143	5.67		1
Pyrogallol	C6H6O3	125.0244	6.31		1
diOH benzoic acid I	C7H6O4	153.0193	9.29		3
3,4-diOH phenylacetic acid	C8H8O4	167.0351	11.14	135.04	1
4-O-methylgallic acid	C8H8O5	183.0299	11.54		1
2,6-dimethoxy benzoic acid	C9H10O4	181.0506	12.08	163.040	1
2-hydroxy hippuric acid	C9H9NO4	194.0459	13.81	178.051	2
diOH benzoic acid II	C7H6O4	153.0193	14.22		3
2,4-diOH benzoic acid	C7H6O4	153.0193	14.57		1
Resorcinol sulfate	C6H6O5S	188.9861	14.87	109.05	2
Benzoic acid	C7H6O2	121.0295	14.89		1
3-O-methylgallic acid	C8H8O5	183.0299	15.07	169.01	2
Daidzein diglucuronide	C27H26O16	605.1148	15.62	429.083/253.051	2
Hippuric acid	C9H9NO3	178.0511	16.53		1
Vanillic acid	C8H8O4	167.0351	17.36		1
3,4-diOH cinnamic acid (caffeic acid)	C9H8O4	179.0351	17.66	135.04	1
3 or 4-OH-phenylpropanoid acid-glucuronide	C15H17O9	341.0879	18.01		3
Phenyl-sulphate	C6H5O4S	172.9918	18.75	97.97	2
Genistein diglucuronide (G-4',7-diG)	C27H26O17	621.1097	19.13	445.08	2
5-(3,4-dihydroxyphenyl)-γ-valerolactone	C11H12O4	207.0663	20.50		1
3-(4-hydroxy phenyl)-1-propionic acid	C9H10O3	165.0557	21.57		1
Daidzein glucuronide sulphate	C21H18O13S	509.0396	21.72	429.083/97.97	2
Daidzein glucuronide I	C21H18O10	429.0827	23.37	253.051	2
4-OH cinnamic acid (p-coumaric acid)	C9H8O3	163.0401	23.45		1
3,5-diMeO-4-OH benzoic acid (syringic acid)	C9H10O5	197.0455	23.56		1
2(4-hydroxy phenyl)propionic acid	C9H10O3	165.0557	23.93		1
3-methoxy-4-hydroxy phenylpropionic acid	C10H12O4	195.0663	24.15		1
5-(3,4-dihydroxyphenyl)-γ-valerolactone-sulphate	C11H12O7S	287.0231	25.33	207.066	2
Resorcinol	C6H6O2	109.0295	25.65		1
Genistein 4'-sulfate-7-glucuronide (G-4'S-7G)	C21H18O14S	525.0342	26.68	349.002/269.045	1
Daidzein glucuronide II	C21H18O10	429.0827	27.17	253.051	2
ferulic acid	C10H10O4	193.0506	27.66		1
Cresol-sulfate	C7H8O4S	187.0071	28.49	97.97	2

Genistein 7-glucuronide (G-7G)	C21H18O11	445.0776	29.19	269.045	2
Genistein 4'-glucuronide-7-sulfate (G-4'G-7S)	C21H18O14S	525.0342	29.95	349.002/269.045	2
5-(3-methoxy-4-hydroxyphenyl)- γ -valerolactone	C12H14O4	221.0819	30.01		1
4-hydroxy phenylacetic acid	C8H8O3	151.0401	30.41		1
3-OH benzoic acid	C7H6O3	137.0244	30.98		1
Genistein 4'-glucuronide (G-4'G)	C21H18O11	445.0776	32.43	269.045	2
Daidzein	C15H10O4	253.0506	38.25		1
Daidzein sulphate	C15H10O7S	333.0073	38.33	253.051/97.97	2
5-hydroxy-equol	C15H14O4	257.0819	39.43		3
4-ethylphenol sulfate	C8H10O4S	201.0225	41.25	97.97	2
Cinnamic acid	C9H8O2	147.0452	41.83		1
Dihydrogenistein	C15H12O5	271.0612	45.58		3
Genistein aglycon	C15H10O5	269.0456	45.86		1
Genistein 4'-sulfate (G-4'S)	C15H10O8S	349.0021	46.04	269.045	1
Genistein 7-sulfate (G-7S)	C15H10O8S	349.0021	46.82	269.045	1

[§] Annotation level

-
- 1 - Unambiguously identified metabolites, checked with standard
 - 2 - Putatively annotated, based on accurate mass and MS/MS fragments
 - 3 - Putatively characterised