

Supplementary Table 1. *m/z* of statistically significantly differing metabolites detected in positive ionisation mode.

ESI mode	Detected <i>m/z</i>	Rt.min	Theoretical MW	Candidate compounds	Log FC [RSV+Q vs HFS]	Log FC [Q vs HFS]	Log FC [RSV vs HFS]	<i>p</i> (Corr)
+	230.0904	7.6833	230.0903	- Pro Asp - 2-Acetyl-5-tetrahydroxybutyl Imidazole - (2S,3'S)-alpha-Amino-2-carboxy-5-oxo-1-pyrrolidinebutanoic acid - Asp Pro - Prolyl-Aspartate - 1-(gamma-Glutamylamino)cyclopropanecarboxylic acid	20.09	0.00	19.73	<i>p</i> < 0.001
			230.0943	- Demethylsuberosin - Pindone - Pondaplin - Osthenol - (S)-Naproxen - 6-O-Methyleuparin - Demethylbatatasin IV - Dihydroresveratrol - Aucuparin - NOPM - Kawain				
			230.0977	- S-methylcaptopril				
+	315.0281	5.0483	315.0274	- Efavirenz	18.62	18.23	0.00	<i>p</i> < 0.001
+	453.0596	5.0458	453.0562	- Floxacillin	17.45	16.79	0.00	<i>p</i> < 0.001
			453.0461	- Ammonium alum				
			453.0454	- Riluzolamide glucuronide				
			453.0433	- Glucoerysolin				
+	290.0463	5.0483	290.0419	- Brompheniramine (didemethylated)	17.39	16.95	0.00	<i>p</i> < 0.001
			290.0403	- Sedoheptulose 7-phosphate - Sedoheptulose 1-phosphate - D-glycero-D-manno-Heptose 7-phosphate				
			290.0548	- 1-[4,9-Dihydro-2-(methylthio)-1,3-thiazino[6,5-b]indol-4-yl]-2-propanone				
+	318.9994	5.0483	318.9908	- 5-Trifluoromethyl-2,4-disulfamoylaniline	16.68	16.31	0.00	<i>p</i> < 0.001

Supplementary Table 1. Continued

ESI mode	Detected <i>m/z</i>	Rt.min	Theoretical MW	Candidate compounds	Log FC [RSV+Q vs HFS]	Log FC [Q vs HFS]	Log FC [RSV vs HFS]	<i>p</i> (Corr)
+	179.0574	5.0440	179.0582	- 5,8-Dihydroxy-3,4-dihydrocarbostyryl - p-Acetaminobenzoic acid - 4-Oxo-4-(3-pyridyl)-butanoic acid - Adrenochrome - Hippuric acid - N-Acetylanthranilate - 1-(4-Methoxyphenyl)-2-nitroethylene - 2,5,6-Trihydroxy-5,6-dihydroquinoline - Methyl n-formylanthranilate	16.43	10.51	0.00	<i>p</i> < 0.001
			179.0616	- (R)C(R)S-S-Propylcysteine sulfoxide - Cyclohexylsulfamate				
+	230.0897	7.9033	230.0903	- Pro Asp - 2-Acetyl-5-tetrahydroxybutyl Imidazole - (2S,3'S)-alpha-Amino-2-carboxy-5-oxo-1-pyrrolidinebutanoic acid - Asp Pro - Prolyl-Aspartate - 1-(gamma-Glutamylamino)cyclopropanecarboxylic acid	16.21	0.00	16.60	<i>p</i> < 0.001
			230.0943	- Demethylsuberosin - Pindone - Pondaplin - Osthenol - (S)-Naproxen - 6-O-Methyleuparin - Demethylbatatin IV - Dihydroresveratrol - Aucuparin - NOPM - Kawain				
			230.0977	- S-methylcaptopril				
+	283.0786	5.0482	283.0804	- Cucumopine	15.97	12.95	0.00	<i>p</i> < 0.001
			283.0845	- (E)-Avenanthramide D - 4-NAPHTHALIMIDOBUTYRIC ACID - Avenanthramide 1p				
+	291.0043	5.0475	291.012	- Brimonidine	15.94	15.56	0.00	<i>p</i> < 0.001
+	216.9793	5.0467	Not identified		15.67	15.22	0.00	<i>p</i> < 0.001

Supplementary Table 1. Continued

ESI mode	Detected <i>m/z</i>	Rt.min	Theoretical MW	Candidate compounds	Log FC [RSV+Q vs HFS]	Log FC [Q vs HFS]	Log FC [RSV vs HFS]	<i>p</i> (Corr)
+	274.0018	5.0467	274.0041	- 4-Ketoifosfamide - 4-Ketocyclophosphamide	15.57	15.17	0.00	<i>p</i> < 0.001
			273.9995	- L-Iduronate 2-sulfate				
			274.0065	- RG-14620				
			274.009	- 1-Phospho- α -D-galacturonate - 3-Dehydro-L-gulonate 6-phosphate - 6-Phospho-2-dehydro-D-gluconate - D-Glucuronic acid 1-phosphate				
+	591.0908	5.0455	591.081	- WSP-1	15.36	12.69	0.00	<i>p</i> < 0.001
+	454.1317	8.8425	454.1369	- 5-iodo-4-hydroxy-docosa-7Z,10Z,13Z,16Z,19Z-pentaenoic acid delta lactone	14.75	0.00	15.21	<i>p</i> < 0.001
			454.1378	- Met Cys Val Cys - Diferentes péptidos				
			454.1394	- Eupachlorin acetate				
			454.141	- Sirodesmin H				
			454.1416	- Ampelopsin D - trans-delta-Viniferin - epsilon-Viniferin - Gnetin A				
			454.1199	Nap-Met-OH Met-Nap-OH Carfecillin				
			454.1192	Cys Cys Glu Thr Other peptides				
			454.1488	TyrMe-His-OH His-TyrMe-OH				
+	324.0258	7.6991	324.0246	- 5-O-(1-Carboxyvinyl)-3-phosphoshikimate	13.93	0.00	17.33	<i>p</i> < 0.001
			324.0272	- Dorzolamide				
			324.032	- Chlorobenzilate				
			324.0359	Arabinose Uridinemonophosphate Arabinoside uridinemonophosphate Uridine monophosphate (UMP) Uridine 2'-phosphate Pseudouridine 5'-phosphate 3'-UMP				

Supplementary Table 1. Continued

ESI mode	Detected <i>m/z</i>	Rt.min	Theoretical MW	Candidate compounds	Log FC [RSV+Q vs HFS]	Log FC [Q vs HFS]	Log FC [RSV vs HFS]	<i>p</i> (Corr)
+	156.0503	3.9633	156.0535	- Imidazole lactate - 4-Imidazolone-5-propionic acid - (S)-3-(Imidazol-5-yl)lactate - N-Nitrosoguvacine - 1-Imidazolelactic acid	10.63	-2.39	13.01	<i>p</i> < 0.001
+	135.0516	4.8364	135.0532	- 2-Hydroxymethylserine - 4-Hydroxy-L-threonine - (+)-threo-2-Amino-3,4-dihydroxybutanoic acid	9.30	13.93	9.28	<i>p</i> = 0.043
			135.0545	- Adenine - 4-(Hydroxymethyl)benzenediazonium(1+)				
			534.2631	- GV 150013X - Pyrophaeophorbide a - Pyropheophorbide a				
			534.2584	- Arg Lys Glu Cys - Diferentes péptidos				
			534.2577	- ANTIMYCIN A (A1 shown)				
			534.2663	- His Asn Lys His - Other peptides				
			534.2676	- 7,8-Dihydrovomifoliol 9-[rhamnosyl-(1->6)-glucoside] - 3-Hydroxy-beta-ionol 3-[glucosyl-(1->6)-glucoside]				
			534.255	- His Glu His Ile - Diferentes péptidos				
			534.2696	- Arg Thr Cys Arg - Diferentes péptidos				
534.2524	- 2-O-Methyl-L-fucose							
+	419.1571	4.2100	419.1652	- Asn Thr Asp Ala - Other peptides	5.49	-7.67	5.59	<i>p</i> = 0.016
			419.1475	- Asn Pro Cys Ser				
			419.1434	- 8-Hydroxy-perphenazine - Perphenazine sulfoxide - Perphenazine-N-oxide - 7-Hydroxyperphenazine				

Supplementary Table 1. Continued

ESI mode	Detected <i>m/z</i>	Rt.min	Theoretical MW	Candidate compounds	Log FC [RSV+Q vs HFS]	Log FC [Q vs HFS]	Log FC [RSV vs HFS]	<i>p</i> (Corr)
+	271.2462	9.5800	271.2511	<ul style="list-style-type: none"> - Hexadecanoic acid, 2-amino-, (R)-; (R)-2-Aminohexadecanoic acid - Hexadecanoic acid, 2-amino-, (S) - Hexadecanoic acid, 2-amino-, (1)- - C16 Sphingosine - Myristoyl-EA - 2-amino-hexadecanoic acid - 2-aminohexadecanoic acid - 2S-aminohexadecanoic acid 	2.02	0.07	2.03	<i>p</i> = 0.003
+	427.3569	12.5608	427.3662	<ul style="list-style-type: none"> - (R)-Stearoylcarnitine - DL-Stearoylcarnitine 	1.81	0.25	1.38	<i>p</i> = 0.019
+	470.2701	14.2238	470.2668	<ul style="list-style-type: none"> - Withaferin A - Stigmatellin X - Withanolide A - Methyl lucidenate F - Withanolide - 3β-HYDROXYDEOXODIHYDRODEOXYGEDUNIN 	1.51	0.70	0.18	<i>p</i> = 0.043
			470.274	<ul style="list-style-type: none"> - Leu Glu Pro Ile - Other peptides 				
			470.2645	<ul style="list-style-type: none"> - PG(15:0/0:0) 				
			470.2759	<ul style="list-style-type: none"> - 6-bromo-25-methyl-hexacos-5E,9Z-dienoic acid - 6-bromo-5,9-hexacosadienoic acid - 6-bromo-5E,9Z-hexacosadienoic acid - 6-bromo-24-methyl-pentacos-5E,9Z-dienoic acid 				
			470.2601	<ul style="list-style-type: none"> - Pro Ala Gln Arg - Other peptides 				
			470.2853	<ul style="list-style-type: none"> - Pro Lys Val Gln - Other peptides 				

Supplementary Table 1. Continued

ESI mode	Detected <i>m/z</i>	Rt.min	Theoretical MW	Candidate compounds	Log FC [RSV+Q vs HFS]	Log FC [Q vs HFS]	Log FC [RSV vs HFS]	<i>p</i> (Corr)
+	299.2772	10.5000	299.2824	<ul style="list-style-type: none"> - (8Z,d18:1) sphingosine - 12-amino-octadecanoic acid - 2-amino-octadecanoic acid - Palmitoyl-EA - 5-hydroxy,3E-sphingosine - 2R-aminooctadec-4Z-ene-1,3S-diol - Sphingosine - 3-ketosphinganine - L-threo-Sphingosine C-18 - Palmitoyl Ethanolamide 	1.27	0.00	1.05	<i>p</i> = 0.011
+	285.2613	10.0400	285.2668	<ul style="list-style-type: none"> - anteiso (4E,14-methyl-d16:1) sphingosine - iso (4E,15-methyl-d16:1) sphingosine - Pentadecanoyl-EA - D-erythro-Sphingosine C-17 	1.14	-0.31	1.11	<i>p</i> = 0.002
+	364.218	7.9400	364.225	<ul style="list-style-type: none"> - Insignin A - 3a,11b,21-Trihydroxy-20-oxo-5b-pregnan-18-al - Vanillin 3-(L-menthoxy)propane-1,2-diol acetal - Acetoxy-8-gingerol - Allotetrahydrocortisone - Tetrahydrocortisone - 11beta,17alpha,21-trihydroxypregnenolone - Dihydrocortisol 	0.75	-11.42	1.19	<i>p</i> = 0.009
			364.2111	<ul style="list-style-type: none"> - Ala Phe Lys - Lys Phe Ala - Phe Lys Ala - Lys Ala Phe - Urocortisone - Ala Lys Phe - Phe Ala Lys 				
			364.205	<ul style="list-style-type: none"> 6alpha-Fluoro-11beta,17-dihydroxypregn-4-ene-3,20-dione 9-Fluoro-11beta,16alpha-dihydroxypregn-4-ene-3,20-dione 				
			364.2038	3-(1,1-Dimethyl-2-propenyl)-8-(3-methyl-2-butenyl)xanthyletin				

Supplementary Table 1. Continued

ESI mode	Detected <i>m/z</i>	Rt.min	Theoretical MW	Candidate compounds	Log FC [RSV+Q vs HFS]	Log FC [Q vs HFS]	Log FC [RSV vs HFS]	<i>p</i> (Corr)
+	270.1523	5.2200	270.162	<ul style="list-style-type: none"> - 3beta-hydroxy-estra-5,7,9-trien-17-one - 3-Hydroxyestra-1,3,5(10)-trien-16-one - 8alpha-3beta-hydroxy-estra-1,3,5(10)-trien-17-one - estra-1,3,5(10),7-tetraene-3,17alpha-diol - Estrone - Estra-1,3,5(10),6-tetraen-3,17beta-diol - ESTRA-4,9-DIENE-3,17-DIONE - 8α-3β-hydroxy-estra-1,3,5(10)-trien-17-one - estra-1,3,5(10),7-tetraene-3,17α-diol - Trenbolone - HEXESTROL - 3β-hydroxy-estra-5,7,9-trien-17-one 	0.33	-2.07	-11.44	<i>p</i> = 0.010
+	158.0659	0.6700	158.0691	<ul style="list-style-type: none"> - 4-Methylene-L-glutamine - 5-Hydroxyectoine - 1-(Hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione 	0.25	1.15	-0.07	<i>p</i> = 0.030
+	146.0663	0.6135	146.0691	<ul style="list-style-type: none"> - L-Glutamine - B-ureidoisobutyric acid - Gly Ala - Alanyl-Glycine - D-Glutamine - Isoglutamine - Ala-Gly - Ala Gly 	0.01	0.30	-11.57	<i>p</i> = 0.015
+	318.1517	7.4325	318.1539	<ul style="list-style-type: none"> - Asp Gly Lys - Other peptides 	-1.07	-1.29	-0.51	<i>p</i> = 0.036
318.1555			- Fluvoxamine					
318.1558			- 2-bromopalmitaldehyde					
318.1467			<ul style="list-style-type: none"> - 2-Hydroxyenterodiol - 4-Hydroxyenterodiol - 6-Hydroxyenterodiol - Zearalenone 					

Supplementary Table 1. Continued

ESI mode	Detected m/z	Rt.min	Theoretical MW	Candidate compounds	Log FC [RSV+Q vs HFS]	Log FC [Q vs HFS]	Log FC [RSV vs HFS]	p (Corr)
+	394.0765	7.3117	394.0777	- 5'-Butyrylphosphoridine	-2.28	-0.13	-12.19	p= 0.009
			394.0741	- Diflufenican				
			394.0689	- Prostalidin A - Tetracenomyacin D3 methylester - Tetracenomyacin B3 - Demethyltorosaflavone C				
			394.09	- 9-Hydroxy-4-methoxypsoralen 9-glucoside				
+	330.1512	5.4978	330.1499	- 8-Hydroxyclopropylamine - 2-Hydroxyclopropylamine	-3.19	-12.73	-0.55	p= 0.009
			330.1539	- Ser Ala Gly Pro - Modificados				
			330.1467	- TETRAHYDROSAPPANONE A TRIMETHYL ETHER				
			330.1402	- Desmethyl methotrimeprazine 5-sulfoxide - Pyributicarb				
			330.1387	17alpha-Chloroethynylestradiol				
+	356.3001	14.2962	356.2927	- 3-(2-Heptenyloxy)-2-hydroxypropyl undecanoate - MG(18:1(11E)/0:0/0:0)[rac] - MG(18:1(9Z)/0:0/0:0)[rac] - Heneicosanedioic acid - Stearoyllactic acid - MG(0:0/18:1(11Z)/0:0) - MG(18:1(9Z)/0:0/0:0) - MG(18:1(9Z)/0:0/0:0) - MG(0:0/18:1(9Z)/0:0) - MG(18:1(11Z)/0:0/0:0)	-9.74	-14.58	-2.35	p= 0.008
			356.3079	- 26,27-bisnor-22-dehydro-cholesterol - (-)-Ceriferol 1				
+	240.1919	7.1323		Not identified	-9.94	-9.85	2.58	p= 0.020

Supplementary Table 1. Continued

ESI mode	Detected <i>m/z</i>	Rt.min	Theoretical MW	Candidate compounds	Log FC [RSV+Q vs HFS]	Log FC [Q vs HFS]	Log FC [RSV vs HFS]	<i>p</i> (Corr)
+	366.1125	5.0393	366.1103	- Puerarostan - 3,9-Dihydroxy-1-methoxy-8-prenylcoumestan - Mirificoumestan - Neorautenanol - 3'-Hydroxyalpinumisoflavone 4'-methyl ether - Barpisoiflavone C - Isoglycyrol - Desmodol - Glycyrol - Wampetin - Vellokaempferol 3-methyl ether - 5-Hydroxy-8-(4-hydroxy-3-methoxyphenyl)-2,2-dimethyl-2H,6H-benzo[1,2-b:5,4-b']dipyrans-6-one - Racemoflavone - Derrubone - Glycyrrhizaisoflavone B	-11.45	-9.10	0.00	<i>p</i> = 0.011
			366.1191	- Ridogrel				
			366.1209	- Gly Ser Thr Cys - Other peptides				
			366.1216	- N-Caffeoyltryptophan				
			366.1032	- Met Asn Cys - Other peptides				
			366.1023	- Atovaquone				
			366.1234	- 3''-Chloro-3''-deoxytriphasiol				
			665.3047	- Natamycin				
+	665.3043	15.4793	665.2962	- Trp Gln Phe Trp - Other peptides	-12.80	-10.31	-0.32	<i>p</i> = 0.010

Supplementary Table 1. Continued

ESI mode	Detected <i>m/z</i>	Rt.min	Theoretical MW	Candidate compounds	Log FC [RSV+Q vs HFS]	Log FC [Q vs HFS]	Log FC [RSV vs HFS]	<i>p</i> (Corr)
+	452.3176	14.5188	452.3102	<ul style="list-style-type: none"> - 24,24-difluoro-1α,25-dihydroxyvitamin D3 / 24,24-difluoro-1α,25-dihydroxycholecalciferol - 4,4-difluoro-1α,25-dihydroxyvitamin D3 / 4,4-difluoro-1α,25-dihydroxycholecalciferol - 23,23-difluoro-1α,25-dihydroxyvitamin D3 / 23,23-difluoro-1α,25-dihydroxycholecalciferol - (5Z)-4,4-difluoro-1α,25-dihydroxyvitamin D3 / (5Z)-4,4-difluoro-1α,25-dihydroxycholecalciferol - PA(O-20:0/0:0) 	-12.99	-8.04	0.31	<i>p</i> = 0.021
			452.329	<ul style="list-style-type: none"> - 3-OXOURSAN (28-13)OLIDE - Tyromycic acid - VD 2736 - 3-Oxo-12,18-ursadien-28-oic acid - (17Z)-1α,25-dihydroxy-26,27-dimethyl-17,20,22,22,23,23-hexadehydro-24a-homovitamin D3 / (17Z)-1α,25-dihydroxy-26,27-dimethyl-17,20,22,22,23,23-hexadehydro-24a-homocholecalciferol - (17E)-1α,25-dihydroxy-26,27-dimethyl-17,20,22,22,23,23-hexadehydro-24a-homovitamin D3 / (17E)-1α,25-dihydroxy-26,27-dimethyl-17,20,22,22,23,23-hexadehydro-24a-homocholecalciferol - 1α,25-dihydroxy-26,27-dimethyl-20,21,22,22,23,23-hexadehydro-24a-homovitamin D3 / 1α,25-dihydroxy-26,27-dimethyl-20,21,22,22,23,23-hexadehydro-24a-homocholecalciferol - (22E,24E,24bE)-1α,25-dihydroxy-22,23,24,24a,24b,24c-hexadehydro-24a,24b,24c-trihomovitamin D3 / (22E,24E,24bE)-1α,25-dihydroxy-22,23,24,24a,24b,24c-hexadehydro-24a,24b,24c-trihomocholecalciferol - VD 2728 				

Supplementary Table 1. Continued

ESI mode	Detected <i>m/z</i>	Rt.min	Theoretical MW	Candidate compounds	Log FC [RSV+Q vs HFS]	Log FC [Q vs HFS]	Log FC [RSV vs HFS]	<i>p</i> (Corr)
+	326.1272	9.8175	326.1267	- Scriptaid	-14.37	-4.93	-9.62	<i>p</i> = 0.032
			326.1298	- Clozapine				
			326.1226	- 6,7-Dimethyl-8-(1-D-ribityl)lumazine				
			326.1318	- 2,2,4-Trimethyl-3-(4-fluorophenyl)-2H-1-benzopyran-7-ol acetate				
			326.1213	- Scillabiose - 2-O-a-L-Fucopyranosyl-galactose - Rutinose - beta-D-Galactosyl-(1->4)-L-rhamnose - 3-O-a-L-Fucopyranosyl-D-glucose - 2-O-alpha-L-Rhamnopyranosyl-D-glucopyranose - Robinobiose				
			326.1339	- Asn Gly His - Other peptides				
			326.1186	- 3-Hydroxydesloratadine - 2H-Benzo[5,6]cyclohepta[1,2-b]pyridin-2-one, 8-chloro-1,5,6,11-tetrahydro-11-(4-piperidinylidene)- - 5H-Benzo[5,6]cyclohepta[1,2-b]pyridin-5-ol, 8-chloro-6,11-dihydro-11-(4-piperidinylidene)- - 5H-Benzo[5,6]cyclohepta[1,2-b]pyridin-6-ol, 8-chloro-6,11-dihydro-11-(4-piperidinylidene)-				
			326.1366	- 4-(4-Hydroxyphenyl)-2-butanone glucoside - Citrusin C - Hinokitiol glucoside				
			326.1365	- Tetranor-PGEM - 1-Methoxy-3-(4-hydroxyphenyl)-2E-propenal 4'-glucoside				

Supplementary Table 1. Continued

ESI mode	Detected m/z	Rt.min	Theoretical MW	Candidate compounds	Log FC [RSV+Q vs HFS]	Log FC [Q vs HFS]	Log FC [RSV vs HFS]	p (Corr)
+	466.3325	14.8791	466.3294	<ul style="list-style-type: none"> - 3alpha,7alpha,12alpha,22S-tetrahydroxy-5beta-cholestan-26-oic acid - (25S)-3alpha,7alpha,12alpha,24R-tetrahydroxy-5beta-cholestan-26-oic acid - (25S)-2beta,3alpha,7alpha,12alpha-tetrahydroxy-5beta-cholestan-26-oic acid - (25R)-1beta,3alpha,7alpha,12alpha-tetrahydroxy-5beta-cholestan-26-oic acid - 3alpha,7alpha,22S-trihydroxy-5alpha-cholestan-26-oic acid - 3alpha,7alpha,12alpha,26-tetrahydroxy-5alpha-cholestan-27-oic acid - (25R)-3alpha,7alpha,12alpha,24R-tetrahydroxy-5beta-cholestan-26-oic acid - (25S)-3alpha,7alpha,12alpha,24S-tetrahydroxy-5beta-cholestan-26-oic acid - 3alpha,7alpha,16alpha,24R-Tetrahydroxy-5beta-cholestan-26-oic acid - 3alpha,7alpha,12alpha,16alpha-Tetrahydroxy-5beta-cholestan-26-oic acid - 3alpha,7alpha,16alpha,22S-Tetrahydroxy-5beta-cholestan-26-oic acid - 3alpha,7alpha,15alpha,22S-Tetrahydroxy-5beta-cholestan-26-oic acid - (25R)-3alpha,7alpha,12alpha,24S-tetrahydroxy-5beta-cholestan-26-oic acid - 3alpha,7alpha,12alpha,26-Tetrahydroxy-5beta-cholestan-27-oic acid - 3alpha,7alpha,12alpha,25-Tetrahydroxy-5beta-cholestan-26-oic acid - 3alpha,6alpha,7alpha,12alpha-Tetrahydroxy-5beta-cholestan-26-oic acid - 1β,3α,7α,12α-Tetrahydroxy-5β-cholestan-26-oic acid - 3α,6α,7α,12α-Tetrahydroxy-5β-cholestan-26-oic acid - 3α,7α,12α,23-Tetrahydroxy-5β-cholestan-26-oic acid - 3α,7α,12α,24-Tetrahydroxy-5α-cholestan-26-oic acid - 2β,3α,7α,12α-Tetrahydroxy-5β-cholestan-26-oic acid - 3α,7α,12α,22-Tetrahydroxy-5β-cholestan-26-oic acid - 3α,7α,12α,25-Tetrahydroxy-5β-cholestan-26-oic acid - 2beta,3alpha,7alpha,12alpha-Tetrahydroxy-5beta-cholestan-26-oic acid - 1beta,3alpha,7alpha,12alpha-Tetrahydroxy-5beta-cholestan-26-oic acid - Varanic acid - 3alpha,7alpha,12alpha,23-Tetrahydroxy-5beta-cholestan-26-oic acid - 3alpha,7alpha,12alpha,24-Tetrahydroxy-5alpha-cholestan-26-oic acid - 3alpha,7alpha,12alpha,22-Tetrahydroxy-5beta-cholestan-26-oic acid - 24,24-difluoro-1α,25-dihydroxy-24a-homovitamin D3 / 24,24-difluoro-1α,25-dihydroxy-24a-homocholecalciferol 	-14.73	-12.27	-4.54	p= 0.009
			466.3258	- 24,24-difluoro-1α,25-dihydroxy-24a-homovitamin D3 / 24,24-difluoro-1α,25-dihydroxy-24a-homocholecalciferol				
			466.3447	<ul style="list-style-type: none"> - 2,3-epoxyphyloquinone - (17Z)-1α,25-dihydroxy-26,27-dimethyl-17,20,22,22,23,23-hexadehydro-24a,24b-dihomovitamin D3 / (17Z)-1α,25-dihydroxy-26,27-dimethyl-17,20,22,22,23,23-hexadehydro-24a,24b-dihomocholecalciferol 				

Supplementary Table 1. Continued

ESI mode	Detected <i>m/z</i>	Rt.min	Theoretical MW	Candidate compounds	Log FC [RSV+Q vs HFS]	Log FC [Q vs HFS]	Log FC [RSV vs HFS]	<i>p</i> (Corr)
+	632.117	5.0455	632.1132	- UDP-2,4-bis(acetamido)-2,4,6-trideoxy-beta-L-altropyranose	17.45	16.79	0.00	<i>p</i> < 0.0001
			632.1013	- 8-C-Ascorbylepigallocatechin 3-gallate - Myricetin 7-(6''-galloylglucoside) - Myricetin 3-(2''-galloylglucoside) - Myricetin 3-(6''-galloylgalactoside) - Myricetin 3-(6''-galloylglucoside) - Myricetin 3-(2''-galloylgalactoside)				
+	407.1281	6.1975	407.1362	- Glu Met Glu - gamma-L-Glutamyl-gamma-L-glutamyl-L-methionine - Glu Glu Met - Met Glu Glu - 8-Carboxymethyldihydrochelerythrine	14.93	0.00	14.93	<i>p</i> < 0.0001
			407.1369	- 8-Carboxymethyldihydrochelerythrine				
			407.1181	- Sitagliptin				
			407.1434	- YS121				

Statistical analyses were performed using One-Way ANOVA followed by Tukey range test and *p* values were corrected by Benjamini-Hochberg procedure. ESI, electrospray ionization mode; Rt, retention time; MW, molecular weight; HFS, high fat sucrose diet-fed control rats; RSV, supplemented with 15 mg/kg BW/day of *trans*-resveratrol; Q, supplemented with 30 mg/kg BW/day of quercetin; RSV + Q, supplemented with a combination of *trans*-resveratrol and quercetin at the same doses; Log FC, log₂ value of fold change.