

Supplementary information

Comparison of the individual sulfated metabolome between plasma and urine samples

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Supplementary figure

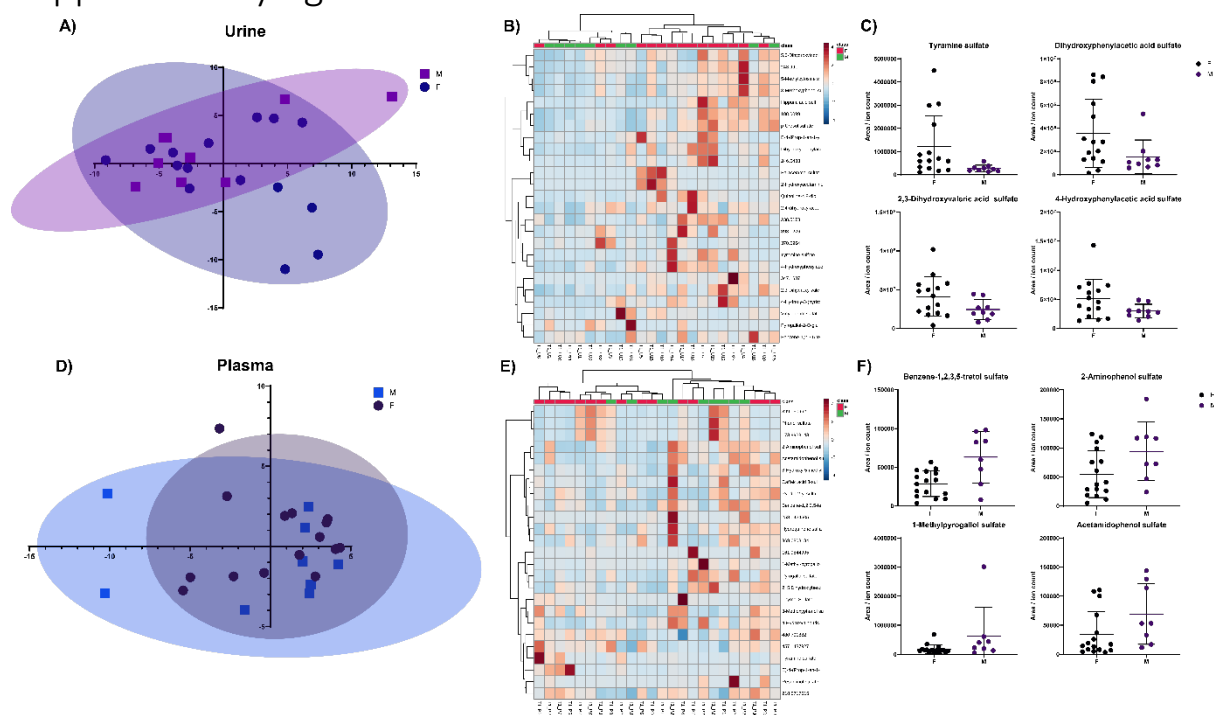


Fig. S1 - Gender effect of the sulfatome. A) Principal component analysis according to gender in urine. B) Heatmap with stratification of the samples for the top 25 sulfated metabolites in urine. C) Mass spectrometric values for the top 4 metabolites altered in urine. D) Principal component analysis according to gender in plasma. E) Heatmap with stratification of the samples on the top 25 sulfated metabolites in plasma. F) Mass spectrometric values for the top 4 metabolites altered in plasma.

Supplementary tables

Table S1 – Full in-house library of sulfates arranged by molecular weight.

Name	Chemical formula	Experimental [M-H] ⁻	Theoretical [M-H] ⁻	ppm difference	RT /min
		161.9859			5.44
Phenol sulfate	C ₆ H ₅ O ₄ S ⁻	172.9905	172.9914	5.20	6.63
Pyridin-2-yl sulfate	C ₅ H ₄ NO ₄ S ⁻	173.9867	173.9867	0	5.15
Pyridin-3-yl sulfate	C ₅ H ₄ NO ₄ S ⁻	173.9859	173.9867	4.60	2.75
		173.9939			6.96
p-Cresol sulfate	C ₇ H ₇ O ₄ S ⁻	187.0061	187.0071	5.35	8.65
Benzyl alcohol sulfate	C ₇ H ₇ O ₄ S ⁻	187.0071	187.0071	0	8.21
		187.9778			7.52
Aminophenol sulfate 1	C ₆ H ₆ NO ₄ S ⁻	188.0011	188.0023	6.38	3.33
Aminophenol sulfate 2	C ₆ H ₆ NO ₄ S ⁻	188.0015	188.0023	4.26	4.19
Aminophenol sulfate 3	C ₆ H ₆ NO ₄ S ⁻	188.0015	188.0023	4.26	4.5
		188.0099			8.75
Resorcinol sulfate	C ₆ H ₅ O ₅ S ⁻	188.9856	188.9863	3.70	5.6
Hydroquinone sulfate	C ₆ H ₅ O ₅ S ⁻	188.9860	188.9863	1.59	4.58
Pyrocatechol sulfate	C ₆ H ₅ O ₅ S ⁻	188.9864	188.9863	0.53	8.4
		189.0030			4.48
Cytosine sulfate	C ₄ H ₄ N ₃ O ₄ S ⁻	189.9890	189.9928	20.00	6.42
6-Hydroxycyclohexa-1,3 dien-yl sulfate	C ₆ H ₇ O ₅ S ⁻	191.0020	191.0020	0.00	5.69
		191.0216			2.51
		191.9684			2.5
4-Cyanophenyl sulfate	C ₇ H ₇ NO ₄ S ⁻	197.9857	197.9867	5.05	7.53
Vinylphenol sulfate 1	C ₈ H ₇ O ₄ S ⁻	199.0059	199.0071	6.03	5.01
Vinylphenol sulfate 2	C ₈ H ₇ O ₄ S ⁻	199.0067	199.0071	2.01	9.79
4-Ethylphenylsulfate	C ₈ H ₉ O ₄ S ⁻	201.0218	201.0227	4.48	10.38

		202.9990			7.18
4-Methoxyphenol sulfate	C ₇ H ₇ O ₅ S ⁻	203.0013	203.0020	3.45	7.18
3-Hydroxy-5-methylphenyl sulfate	C ₇ H ₇ O ₅ S ⁻	203.0014	203.0020	2.96	8.65
2-Methoxyphenol sulfate	C ₇ H ₇ O ₅ S ⁻	203.0023	203.0020	1.48	7.54
3-Methoxyphenol sulfate	C ₇ H ₇ O ₅ S ⁻	203.0024	203.0020	1.97	8.29
		203.9724			5.49
Aminohydroxyphenyl sulfate	C ₆ H ₆ NO ₅ S ⁻	203.9960	203.9972	5.88	2.99
5-Methylcytosine sulfate	C ₅ H ₆ N ₃ O ₄ S ⁻	204.0047	204.0084	18.14	8.25
		204.9801			3.78
3-Hydroxy-2-methyl-4-pyrone sulfate	C ₆ H ₅ O ₆ S ⁻	204.9812	204.9812	0	5.30
Pyrogallol sulfate 1	C ₆ H ₅ O ₆ S ⁻	204.9804	204.9812	3.90	6.44
Pyrogallol sulfate 2	C ₆ H ₅ O ₆ S ⁻	204.9805	204.9812	3.42	5.69
Pyrogallol sulfate 3	C ₆ H ₅ O ₆ S ⁻	204.9807	204.9812	2.44	5.81
Pyrogallol sulfate 4	C ₆ H ₅ O ₆ S ⁻	204.9809	204.9812	1.46	5.31
4,5-Dimethyl-3-hydroxy-2,5-dihydrofuran-2-one sulfate	C ₆ H ₇ O ₆ S ⁻	206.9969	206.9969	0	
5,6-Dihydroxycyclohexa-1,3 dien-1 -yl sulfate	C ₆ H ₇ O ₆ S ⁻	206.9965	206.9969	1.93	6.24
		210.9733			6.71
Indoxyl 3 sulfate	C ₈ H ₇ NO ₄ S ⁻	212.0017	212.0023	2.83	7.94
Indoxyl sulfate	C ₈ H ₇ NO ₄ S ⁻	212.0018	212.0023	2.36	8.16
2,3-Dihydroxy-valeric acid sulfate	C ₅ H ₉ O ₇ S ⁻	213.0056	213.0074	8.45	7.24
E-4-(Prop-1-en-1-yl)phenyl sulfate	C ₉ H ₉ O ₄ S ⁻	213.0215	213.0227	5.63	11.12
Chavicol sulfate	C ₉ H ₉ O ₄ S ⁻	213.0215	213.0227	5.63	10.89
2-Hydroxyacetophenone sulfate	C ₈ H ₇ O ₅ S ⁻	215.0020	215.0020	0	
Vinylbenzene diol sulfate	C ₈ H ₇ O ₅ S ⁻	215.0012	215.0020	3.72	9.35
2-Acetylphenyl sulfate	C ₈ H ₇ O ₅ S ⁻	215.0016	215.0020	1.86	7.69
Hypoxanthine sulfate	C ₅ H ₃ N ₄ O ₄ S ⁻	214.9880	214.9880	0	2.58
Tyramine sulfate	C ₈ H ₁₀ NO ₄ S ⁻	216.0327	216.0336	4.17	5.1
4-Hydroxybenzoic acid sulfate	C ₇ H ₅ O ₆ S ⁻	216.9802	216.9812	4.61	6.87
Hydroxybenzoic acid sulfate 1	C ₇ H ₅ O ₆ S ⁻	216.9803	216.9812	4.15	6.18

2-Hydroxybenzoic acid sulfate	$C_7H_5O_6S^-$	216.9804	216.9812	3.69	6.63
3-Hydroxybenzoic acid sulfate	$C_7H_5O_6S^-$	216.9804	216.9812	3.69	7.10
Hydroxybenzoic acid sulfate 2	$C_7H_5O_6S^-$	216.9805	216.9812	3.23	7.52
2-(2-Hydroxyethyl)phenyl hydrogen sulfate	$C_8H_9O_5S^-$	217.0164	217.0176	5.53	6.82
Creosol sulfate	$C_8H_9O_5S^-$	217.0171	217.0176	2.30	9.88
		218.873			1.36
		218.905			1.32
		218.9959			5.82
		218.996			6.17
1-Methyl-pyrogallol-3-O-sulfate	$C_7H_7O_6S^-$	218.9961	218.9961	218.9969	3.65
2, 5 Dihydroxybenzyl alcohol sulfate	$C_7H_7O_6S^-$	218.9961	218.9961	218.9969	3.65
		218.9968			5.5
Benzene-1,2,3,5-tetrol sulfate	$C_6H_5O_7S^-$	220.9754	220.9761	3.17	6.07
Quinolin-2-yl hydrogen sulfate	$C_9H_6NO_4S^-$	224.0013	224.0023	4.46	7.71
		227.0215			5.56
p-Butenylphenol sulfate	$C_{10}H_{11}O_4S^-$	227.0376	227.0384	3.52	11.97
5,6-Dihydroxyindole sulfate 1	$C_8H_6NO_5S^-$	227.9969	227.9972	1.32	6.64
5,6-Dihydroxyindole sulfate 2	$C_8H_6NO_5S^-$	227.9969	227.9972	1.32	6.1
Methoxy-vinylphenol sulfate 1	$C_9H_9O_5S^-$	229.0168	229.0176	3.49	8.15
Methoxy-vinylphenol sulfate 2	$C_9H_9O_5S^-$	229.0168	229.0176	3.49	9.15
Methoxy-vinylphenol sulfate 3	$C_9H_9O_5S^-$	229.0169	229.0176	3.06	10.46
Methoxy-vinylphenol sulfate 4	$C_9H_9O_5S^-$	229.0171	229.0176	2.18	9.27
Thymol sulfate	$C_{10}H_{13}O_4S^-$	229.0535	229.0540	2.18	12.43
		229.9958			6.05
Paracetamol sulfate	$C_8H_8NO_5S^-$	230.0118	230.0129	7.78	6.25
Acetamidophenol sulfate 1	$C_8H_8NO_5S^-$	230.0127	230.0129	0.87	8.29
Acetamidophenol sulfate 2	$C_8H_8NO_5S^-$	230.0130	230.0129	0.43	7.42
N-Methyltyramine sulfate	$C_9H_{12}NO_4S^-$	230.0493	230.0493	0	7.56
		230.0487			5.31

4-Hydroxyphenylacetic acid sulfate	C ₈ H ₇ O ₆ S	230.9960	230.9969	3.90	6.89
3-Hydroxyphenylacetic acid sulfate	C ₈ H ₇ O ₆ S	230.9962	230.9969	3.03	7.11
2,4 dihydroxy acetophenone sulfate 2	C ₈ H ₇ O ₆ S	230.9964	230.9969	2.16	7.55
Vanillin 4-sulfate	C ₈ H ₇ O ₆ S	230.9965	230.9969	1.73	8.14
Mandelic acid sulfate	C ₈ H ₇ O ₆ S	230.9969	230.9969	0	7.33
2-(4-Methoxyphenyl)ethyl hydrogen sulfate	C ₉ H ₁₁ O ₅ S ⁻	231.0324	231.0333	3.90	10
(4-Ethyl-2-methoxyphenyl)oxidanesulfonic acid	C ₉ H ₁₁ O ₅ S ⁻	231.0328	231.0333	2.16	11.3
5-Aminosalicylic acid sulfate	C ₉ H ₁₁ O ₅ S ⁻	231.9921	231.9921	0	5.98
		232.0192			4.43
Dopamine-3-sulfate	C ₈ H ₁₀ NO ₅ S ⁻	232.0272	232.0285	5.60	4.98
Dopamine-4-sulfate	C ₈ H ₁₀ NO ₅ S ⁻	232.0276	232.0285	3.88	5.12
Hydroxytyrosol sulfate	C ₈ H ₉ O ₆ S ⁻	233.0115	233.0125	4.29	6.63
4-Hydroxy-3-(hydroxymethyl)benzyl sulfate	C ₈ H ₉ O ₆ S ⁻	233.0115	233.0125	4,29	6.22
Methoxybenzene triol sulfate 1	C ₇ H ₇ O ₇ S ⁻	234.9908	234.9918	4.26	5.45
Methoxybenzene triol sulfate 2	C ₇ H ₇ O ₇ S ⁻	234.9909	234.9918	3.83	5.19
	C ₁₀ H ₈ NO ₄ S ⁻	238.0173			6.74
		239.8787			1.3
Indole carboxylic acid Sulfate	C ₉ H ₆ NO ₅ S ⁻	239.9962	239.9972	4.17	8.54
Quinoline-4,8-diol sulfate	C ₉ H ₆ NO ₅ S ⁻	239.9965	239.9972	2.92	8.15
		240.9807			7.93
4-Hydroxycoumarin sulfate	C ₉ H ₅ O ₆ S ⁻	240.9812	240.9812	0	9.36
Umbelliferone sulfate	C ₉ H ₅ O ₆ S ⁻	240.9812	240.9812	0	7.89
		241.0008			8.15
		241.9756			2.69
		241.9757			2.37
		242.0120			7.01
7-Hydroxy-3,4-dihydroquinolin-2-yl sulfate	C ₉ H ₈ NO ₅ S ⁻	242.0123	242.0129	2.48	8.21
trans-3-Hydroxycinnamic acid sulfate	C ₉ H ₇ O ₆ S ⁻	242.9958	242.9969	4.53	8.01
trans-4-Hydroxycinnamic acid sulfate	C ₉ H ₇ O ₆ S ⁻	242.9967	242.9969	0.82	8.52

Raspberry ketone sulfate	$C_{10}H_{11}O_5S^-$	243.0333	243.0333	0	8.34
4-Phenylbutanic acid O sulfate 1	$C_{10}H_{11}O_5S^-$	243.0319	243.0333	5.76	11.37
4-Phenylbutanic acid O sulfate 2	$C_{10}H_{11}O_5S^-$	243.0326	243.0333	2.88	10.85
		243.9910			6.1
		245.0120			4.96
D-3-Phenyllactic acid sulfate	$C_9H_9O_6S^-$	245.0125	245.0125	0	10.2
Phloretic acid sulfate	$C_9H_9O_6S^-$	245.0127	245.0125	0.82	8.97
3-(3-Hydroxyphenyl)propionic acid sulfate	$C_9H_9O_6S^-$	245.0128	245.0125	0	8.03
2-tert-Butylhydroquinone sulfate	$C_{10}H_{13}O_5S^-$	245.0483	245.0489	2.45	10.1
		245.0484			8.86
2,6-Dihydroxybenzothiazole sulfate 1	$C_7H_4NO_5S_2^-$	245.9524	245.9536	4.88	7.49
2,6-Dihydroxybenzothiazole sulfate 2	$C_7H_4NO_5S_2^-$	245.9527	245.9536	3.66	7.78
2-Hydroxyacetaminophen sulfate	$C_8H_8NO_6S^-$	246.0070	246.0078	3.25	5.97
		246.0432			5.49
		246.0433			2.53
Dihydroxyphenylacetic acid sulfate	$C_8H_7O_7S^-$	246.9909	246.9918	3.64	6.04
Vanillic acid sulfate	$C_8H_7O_7S^-$	246.9912	246.9918	2.43	6.67
5-Methoxysalicylic acid sulfate	$C_8H_7O_7S^-$	246.9918	246.9918	0	7.58
Homovanillyl alcohol sulfate 1	$C_9H_{11}O_6S^-$	247.0273	247.0282	3.64	4.95
Homovanillyl alcohol sulfate 2	$C_9H_{11}O_6S^-$	247.0278	247.0282	1.62	7.62
2-Biphenylol sulfate	$C_{12}H_9O_4S^-$	249.0233	249.0227	2.41	11.72
		249.9890			2.9
		254.9435			7
		255.0182			8.1
Serotonin sulfate	$C_{10}H_{11}N_2O_4S^-$	255.0445	255.0445	0	5.92
5-hydroxytryptophol sulfate	$C_{10}H_{10}O_5S^-$	256.0272	256.0285	5.08	6.89
		256.0280			7.76
		256.9754			7.72
Hippuric acid sulfate	$C_9H_8NO_6S^-$	258.0069	258.0078	3.47	6.37

		258.0437			5.18
4-Hydroxyphenylpyruvic acid sulfate	C ₁₀ H ₉ O ₇ S ⁻	258.9915	258.9918	1.16	7.79
Caffeic acid sulfate 1	C ₁₀ H ₉ O ₇ S ⁻	258.9915	258.9918	1.16	7.54
Caffeic acid sulfate 2	C ₁₀ H ₉ O ₇ S ⁻	258.9918	258.9918	0	8.06
Propylparaben sulfate	C ₁₀ H ₁₁ O ₆ S ⁻	259.0271	259.0282	4.25	10.92
L-Tyrosine-O-sulfate	C ₉ H ₁₀ NO ₆ S ⁻	260.0236	260.0234	0.77	5
3,4 Dihydrocinnamic acid sulfate	C ₉ H ₉ O ₇ S ⁻	261.0067	261.0074	2.68	6.57
Homovanillic acid sulfate	C ₉ H ₉ O ₇ S ⁻	261.0070	261.0074	1.53	7.16
4-Hydroxy-3-methoxyphenylacetic acid sulfate	C ₉ H ₉ O ₇ S ⁻	261.0074	261.0074	0	7.53
Dihydroxyconiferyl alcohol sulfate	C ₁₀ H ₁₃ O ₆ S ⁻	261.0435	261.0438	1.15	8.7
		263.0582			12.78
		267.9578			4.5
		268.9425			6.42
[(6-Hydroxy-1-oxo-1H-isochromen-3-yl)methoxy]sulfonic acid	C ₁₀ H ₇ O ₇ S ⁻	270.9917	270.9918	0.37	7.94
Ferulic acid 4-O-sulfate	C ₁₀ H ₉ O ₇ S ⁻	273.0070	273.0074	1.47	8
Isoferulic acid sulfate	C ₁₀ H ₉ O ₇ S ⁻	273.0073	273.0074	0.37	8.16
3-Hydroxyhippuric acid sulfate	C ₉ H ₈ NO ₇ S ⁻	274.0018	274.0027	3.28	7
4-Hydroxyhippuric acid sulfate	C ₉ H ₈ NO ₇ S ⁻	274.0030	274.0027	1.09	6.24
		274.0385			7.05
Syringic acid sulfate		277.0024			6.99
Harmalol sulfate	C ₁₂ H ₁₁ N ₂ O ₄ S ⁻	279.0541	279.0445	34.40	9.59
		281.0603			8.3
		281.0699			10.42
3-Butylidene-7-hydroxyphthalide sulfate	C ₁₂ H ₁₁ O ₆ S ⁻	283.0277	283.0282	1.77	9.74
Xanthurenic acid 8-O-sulfate	C ₁₀ H ₆ NO ₇ S ⁻	283.9863	283.9870	2.46	7.73
		285.0436			11.13
5'-(3',4'-Dihydroxyphenyl)-gamma-valerolactone sulfate 1	C ₁₁ H ₁₁ O ₇ S ⁻	287.0227	287.0231	1.39	8.13
5'-(3',4'-Dihydroxyphenyl)-gamma-valerolactone sulfate 2	C ₁₁ H ₁₁ O ₇ S ⁻	287.0236	287.0231	1.74	7.89
		288.9517			6.82

3-[3-Hydroxy-5-methoxy-4-(sulfooxy)phenyl]prop-2-enoic acid	C ₁₀ H ₉ O ₈ S ⁻	289.0025	289.0024	0.35	8.08
4-Hydroxy-5-(3'-hydroxyphenyl)-valeric acid-3'-O-sulphate	C ₁₁ H ₁₃ O ₇ S ⁻	289.0385	289.0387	0.69	9.7
		291.0005			9.83
		291.0178			7.91
		291.9577			7.39
		292.0227			7.13
		293.9563			7.25
Methyl dioxindole-3-acetate sulfate 1	C ₁₁ H ₁₀ NO ₇ S ⁻	300.0176	300.0183	2.33	7.75
Methyl dioxindole-3-acetate sulfate 2	C ₁₁ H ₁₀ NO ₇ S ⁻	300.0179	300.0183	1.33	7.47
N-Acetylgalactosamine 6-sulfate 1	C ₈ H ₁₅ NO ₉ S ⁻	300.0389	300.0395	2.00	1.71
N-Acetylgalactosamine 6-sulfate 2	C ₈ H ₁₅ NO ₉ S ⁻	300.0390	300.0395	1.67	1.95
Sinapic acid sulfate	C ₁₁ H ₁₁ O ₈ S ⁻	303.0178	303.0180	0.66	8.03
		304.0208			8.05
		305.0331			7.56
		307.9529			6.1
		307.9896			5.5
		307.9925			9.49
		308.0771			6.69
		309.0981			10.9
		309.1008			13.59
		310.9046			8.18
		311.9852			5.11
3-Hydroxyflavone sulfate	C ₁₅ H ₉ O ₆ S ⁻	317.0125	317.0125	0	12.8
		318.0650			9.01
		325.0369			9.36
		325.0399			8.47
		326.9476			6.66
N-acryloyl-3,4-dihydroxy-DL-phenylalanine sulfate	C ₁₂ H ₁₂ NO ₈ S ⁻	330.0291	330.0289	0.61	7.62
Daidzein sulfate	C ₁₅ H ₉ O ₇ S ⁻	333.0065	333.0074	2.70	10.28

8,2'-Dihydroxyflavone sulfate	C ₁₅ H ₉ O ₇ S ⁻	333.0076	333.0074	0.60	8.09
Dihydrodaidzein sulfate	C ₁₅ H ₁₁ O ₇ S ⁻	335.0211	335.0231	5.97	9.55
Tetrahydrodaidzein sulfate	C ₁₅ H ₁₃ O ₇ S ⁻	337.0364	337.0387	6.82	9.23
		337.9631			6.36
3-(2-((3,4-Dihydroxybenzyl)amino)ethyl)phenyl sulfate 1	C ₁₅ H ₁₆ NO ₆ S ⁻	338.0700	338.0704	1.18	11.08
3-(2-((3,4-Dihydroxybenzyl)amino)ethyl)phenyl sulfate 2	C ₁₅ H ₁₆ NO ₆ S ⁻	338.0701	338.0704	0.89	10.85
		338.0809			8.45
		340.9641			7.6
		341.0509			6.79
		342.1014			10.75
		342.9788			4.96
		344.1168			11.18
		347.1687			12.05
		352.0863			11.81
		352.0868			11.65
Dihydronaringenin-O-sulphate	C ₁₅ H ₁₃ O ₈ S ⁻	353.0332	353.0337	1.42	11.07
		353.9584			6.24
		353.9948			5.87
		356.1165			12.7
		356.1171			11.58
		357.1203			11.59
		358.0817			5.41
Nigellic acid sulfate	C ₁₅ H ₁₉ O ₈ S ⁻	359.0806	359.0806	0	11.97
		367.0022			8.06
		369.0269			7.82
		369.0281			8.66
		369.0817			9.79
		370.0964			9.2
		372.1118			9.82

		372.1125			9.46
Enterolactone sulfate	C ₁₈ H ₁₇ O ₇ S ⁻	377.0700	377.0700	0	10.73
		378.1018			12.65
Pyrogallol-2-O-glucuronide sulfate	C ₁₂ H ₁₄ O ₁₂ S ⁻	381.0126	381.0133	1.84	5.69
Enterodiol sulfate	C ₁₄ H ₁₇ N ₆ O ₅ S ⁻	381.1021	381.1013	2.10	10.45
		382.1040			9.38
		388.0506			1.77
		393.0514			9.02
		393.0650			10.37
		398.1276			10.91
		399.0613			7.5
		408.0956			6.89
		425.0118			7.28
		457.0669			7.53
		457.1542			13.72
		470.1116			13.66
		480.7824			1.31
		497.1693			13.71
		497.1697			14.08
		505.0207			6.24
Daidzein-7-glucuronide-4-sulfate	C ₂₁ H ₁₇ O ₁₃ S ⁻	509.0387	509.0395	1.57	8.43
Genistein-7-glucuronide-4-sulfate	C ₂₁ H ₁₇ O ₁₄ S ⁻	525.0336	525.0344	1.52	8.71
Enterolactone glucuronide sulfate	C ₂₄ H ₂₅ O ₁₃ S ⁻	553.1022	553.1021	0.18	9.52
Enterodiol glucuronide sulfate	C ₂₄ H ₂₉ O ₁₃ S ⁻	557.1342	557.1334	1.44	9.39
		563.1878			8.41

Table S2 – Statistical analysis of the sulfates identified in urine according to age groups. Significantly altered metabolites identified in the one-way ANOVA analysis are highlighted in red.

Sulfate	one-way ANOVA	Group I vs Group II	Group I vs Group III	Group II vs Group III
161.9859	0.3182	0.1852	0.4931	0.1797
Phenol sulfate	0.6804	0.8459	0.3461	0.4186
Pyridin-2-yl sulfate	0.7243	0.8031	0.6658	0.3585
173.9939	0.7515	0.6143	0.8792	0.5591
<i>p</i> -Cresol sulfate	0.0398	0.5766	0.0928	0.0252
Aminophenol sulfate 2	0.5510	0.6092	0.5963	0.2794
Aminophenol sulfate 1	0.9378	0.7598	0.7633	0.9449
Aminophenol sulfate 3	0.5560	0.6556	0.2228	0.5245
188.0099	0.0109	0.1807	0.0928	0.0077
Resorcinol sulfate	0.9436	0.7909	0.9760	0.7958
Pyrocatechol sulfate	0.3391	0.1825	0.5256	0.3586
Hydroquinone sulfate	0.3757	0.2410	0.1553	0.8152
189.003	0.3897	0.2756	0.4140	0.5233
Cytosine sulfate	0.8437	0.9723	0.6795	0.5282
6-Hydroxycyclohexa-1,3 dien-yl sulfate	0.9681	0.9352	0.8829	0.7877
4-Cyanophenyl sulfate	0.8814	0.6962	0.6666	0.9635
Vinylphenol sulfate 1	0.9048	0.6997	0.9242	0.7629
Vinylphenol sulfate 2	0.7795	0.6906	0.6267	0.5663
4-Ethylphenylsulfate	0.5889	0.5449	0.3480	0.6145
3-Hydroxy-5-methylphenyl sulfate	0.8869	0.7973	0.8472	0.6103
2-Methoxyphenol sulfate	0.8349	0.9306	0.7000	0.5211
3-Methoxyphenol sulfate	0.0656	0.4679	0.1722	0.0360
203.9724	0.8232	0.7507	0.7703	0.5612
Aminohydroxyphenyl sulfate	0.0006	0.6541	0.0035	0.0023
5-Methylcytosine sulfate	0.0821	0.3960	0.1966	0.0552

Pyrogallol sulfate 4	0.3681	0.8172	0.2984	0.1816
Pyrogallol sulfate 1	0.0015	0.2035	0.0065	0.0096
Pyrogallol sulfate 3	0.3756	0.8408	0.0814	0.2653
5,6-Dihydroxycyclohexa-1,3 dien-1 -yl sulfate	0.5540	0.8672	0.1863	0.3805
Indoxyl 3 sulfate	0.9227	0.8268	0.6431	0.8546
2,3-Dihydroxy-valeric acid sulfate	0.8138	0.8083	0.6847	0.5602
Chavicol sulfate	0.1774	0.1028	0.7388	0.2176
E-4-(Prop-1-en-1-yl)phenyl sulfate	0.5295	0.4494	0.7556	0.2011
Vinylbenzene diol sulfate	0.9848	0.8751	0.9038	0.9799
2-Acetylphenyl sulfate	0.8551	0.7468	0.8333	0.6120
Tyramine sulfate	0.9530	0.8763	0.8788	0.7765
Hydroxybenzoic acid sulfate 3	0.8047	0.5545	0.7523	0.7158
Hydroxybenzoic acid sulfate 2	0.0150	0.6502	0.0278	0.0291
Creosol sulfate	0.6857	0.5110	0.5458	0.9172
2-(2-Hydroxyethyl)phenyl hydrogen sulfate	0.7915	0.6129	0.5168	0.9484
218.873	0.2063	0.1321	0.2988	0.5251
218.905	0.1623	0.1025	0.5099	0.0304
218.9968	0.9546	0.8773	0.7491	0.8723
218.9959	0.9740	0.8536	0.8258	0.9649
218.996	0.9362	0.7288	0.7676	0.9600
1-Methyl-pyrogallol-3-O-sulfate	0.7517	0.9188	0.2903	0.5626
2, 5 Dihydroxybenzyl alcohol sulfate	0.3343	0.5446	0.1261	0.3085
Benzene-1,2,3,5-tetrol sulfate	0.6929	0.5005	0.9084	0.3752
227.0215	0.7235	0.5453	0.8886	0.5811
p-Butenylphenol sulfate	0.8898	0.8444	0.5364	0.7787
5,6-Dihydroxyindole sulfate 1	0.0287	0.1155	0.0195	0.1299
5,6-Dihydroxyindole sulfate 2	0.0049	0.1242	0.0109	0.0245
Methoxy-vinylphenol sulfate	0.4617	0.2180	0.2925	0.7618
Thymol sulfate	0.5668	0.2303	0.9414	0.4069

229.9958	0.3819	0.2715	0.4188	0.0402
Paracetamol sulfate	0.3332	0.1358	0.6972	0.2273
Acetamidophenol sulfate 2	0.2699	0.2568	0.5940	0.1195
Acetamidophenol sulfate 1	0.1155	0.4253	0.2414	0.0649
230.0487	0.4520	0.4171	0.0175	0.7348
2,4 dihydroxy acetophenone sulfate 1	0.4170	0.2355	0.6417	0.3504
4-Hydroxyphenylacetic acid sulfate	0.9882	0.9012	0.9897	0.9100
2,4 dihydroxy acetophenone sulfate 2	0.8847	0.6624	0.8843	0.7390
2-(4-Methoxyphenyl)ethyl hydrogen sulfate	0.8538	0.7013	0.6191	0.8611
(4-Ethyl-2-methoxyphenyl)oxidanesulfonic acid	0.3362	0.1459	0.5299	0.4158
Dopamine-4-sulfate	0.1185	0.1074	0.7330	0.0319
Dopamine-3-sulfate	0.3337	0.1981	0.9047	0.0751
Hydroxytyrosol sulfate	0.1671	0.1332	0.1717	0.9608
4-Hydroxy-3-(hydroxymethyl)benzyl sulfate	0.4398	0.7247	0.2283	0.2325
Methoxybenzene triol sulfate 1	0.5721	0.4963	0.1439	0.4277
Methoxybenzene triol sulfate 2	0.5320	0.3805	0.9926	0.3936
238.0173	0.6855	0.7745	0.6412	0.3423
239.8787	0.0237	0.2805	0.1210	0.0135
Quinoline-4,8-diol sulfate	0.0626	0.0450	0.2125	0.1184
240.9807	0.1130	0.5527	0.2113	0.0583
241.9756	0.8799	0.6325	0.8735	0.7253
241.9757	0.4367	0.3971	0.2267	0.6739
242.0120	0.0466	0.5035	0.1277	0.0391
trans-3-Hydroxycinnamic acid sulfate	0.2887	0.1753	0.4027	0.1914
trans-4-Hydroxycinnamic acid sulfate	0.3035	0.6870	0.3081	0.0728
4-Phenylbutanic acid O sulfate 1	0.2460	0.2553	0.0901	0.4678
243.9910	0.1797	0.2993	0.1042	0.2864
Phloretic acid sulfate 1	0.4728	0.4752	0.2426	0.5647
Phloretic acid sulfate 2	0.7638	0.6359	0.5624	0.7178

2-tert-Butylhydroquinone sulfate	0.2347	0.0498	0.3793	0.1588
2-Hydroxyacetaminophen sulfate	0.3929	0.1264	0.9528	0.2272
246.0433	0.0208	0.7152	0.0751	0.0252
246.0432	0.3784	0.2531	0.4326	0.4554
Dihydroxyphenylacetic acid sulfate	0.2135	0.8986	0.2132	0.1166
Vanillic acid sulfate	0.5363	0.4102	0.2637	0.8662
Homovanillyl alcohol sulfate	0.7202	0.8246	0.6243	0.4450
256.028	0.7377	0.5424	0.5513	0.9595
5-hydroxytryptophol sulfate	0.1323	0.3323	0.2322	0.1064
256.9754	0.3707	0.2699	0.3910	0.5821
Hippuric acid sulfate	0.4019	0.8423	0.2863	0.2542
258.0437	0.8772	0.9023	0.7442	0.6618
Caffeic acid sulfate 1	0.1592	0.4090	0.3133	0.0748
Caffeic acid sulfate 2	0.0078	0.0050	0.0891	0.1534
Propylparaben sulfate	0.2597	0.1321	0.3711	0.1800
L-Tyrosine-O-sulfate	0.8903	0.6410	0.7123	0.9080
3,4 Dihydrocinnamic acid sulfate	0.5768	0.4358	0.4181	0.9264
Homovanillic acid sulfate 1	0.7135	0.4961	0.6239	0.6450
Homovanillic acid sulfate 2	0.2928	0.1728	0.6615	0.1348
Dihydroxyconiferyl alcohol sulfate	0.3705	0.1753	0.3461	0.6949
267.9578	0.5510	0.8808	0.3476	0.3327
268.9425	0.0711	0.1237	0.1045	0.1075
[(6-Hydroxy-1-oxo-1H-isochromen-3-yl)methoxy]sulfonic acid	0.9780	0.8809	0.8393	0.9436
Isoferulic acid sulfate	0.0686	0.0379	0.2124	0.2821
4-Hydroxyhippuric acid sulfate	0.4576	0.2144	0.2945	0.8984
274.0385	0.6659	0.4722	0.9361	0.3399
281.0603	0.2760	0.2138	0.3188	0.6558
281.0699	0.5278	0.4520	0.2034	0.7636

3-Butylidene-7-hydroxyphthalide sulfate	0.9908	0.9178	0.9088	0.9656
5'-(3',4'-Dihydroxyphenyl)-gamma-valerolactone sulfate 1	0.3725	0.2203	0.7769	0.3557
5'-(3',4'-Dihydroxyphenyl)-gamma-valerolactone sulfate 2	0.7409	0.6000	0.7977	0.5139
288.9517	0.2082	0.2234	0.3747	0.1246
4-Hydroxy-5-(3'-hydroxyphenyl)-valeric acid-3'-O-sulphate	0.8848	0.9606	0.5171	0.7012
291.9577	0.6228	0.4443	0.8019	0.5152
293.9563	0.6523	0.3868	0.6660	0.6299
Methyl dioxindole-3-acetate sulfate	0.2289	0.1509	0.8456	0.2223
N-Acetylgalactosamine 6-sulfate	0.1798	0.5957	0.0496	0.1542
Sinapic acid sulfate	0.5687	0.8622	0.1819	0.4076
305.0331	0.1753	0.2012	0.7086	0.1478
307.9529	0.0125	0.9714	0.0485	0.0222
307.9896	0.7576	0.6705	0.7046	0.5360
308.0771	0.6210	0.4080	0.9298	0.3203
309.0981	0.3042	0.6088	0.3140	0.2512
311.9852	0.3247	0.1382	0.9884	0.1464
318.065	0.5074	0.3074	0.2521	0.7727
325.0399	0.5810	0.4446	0.8651	0.4006
326.9476	0.5872	0.6858	0.2632	0.4937
N-acryloyl-3,4-dihydroxy-DL-phenylalanine sulfate	0.5749	0.4116	0.3658	0.9599
3-(2-((3,4-Dihydroxybenzyl)amino)ethyl)phenyl sulfate 1	0.2237	0.2873	0.1759	0.2689
3-(2-((3,4-Dihydroxybenzyl)amino)ethyl)phenyl sulfate 2	0.4883	0.5168	0.3157	0.4570
338.0809	0.3995	0.1842	0.8796	0.2277
340.9641	0.2878	0.2138	0.3439	0.3363

341.0509	0.5632	0.3651	0.9553	0.2929
342.1014	0.8304	0.7961	0.7481	0.5811
344.1168	0.6129	0.7840	0.5512	0.4119
347.1687	0.3340	0.2050	0.5281	0.0887
352.0863	0.4016	0.4305	0.2006	0.5119
352.0868	0.4788	0.8578	0.2327	0.2745
353.9948	0.4690	0.1904	0.9472	0.3357
356.1171	0.9432	0.8625	0.8903	0.7057
357.1203	0.9506	0.8813	0.8906	0.7267
Nigelliacid sulfate	0.5268	0.5918	0.5870	0.2698
369.0817	0.6003	0.7777	0.3438	0.3412
370.0964	0.3067	0.7012	0.2675	0.0954
372.1118	0.8938	0.7099	0.9615	0.5911
372.1125	0.9073	0.6931	0.9608	0.6525
Enterolactone sulfate	0.0936	0.3640	0.2833	0.0246
378.1018	0.5749	0.9063	0.2397	0.3548
Pyrogallol-2-O-glucuronide sulfate	0.4848	0.8235	0.0782	0.2995
381.1021	0.2510	0.2909	0.2746	0.2191
388.0506	0.2837	0.2492	0.6548	0.1163
393.0514	0.0805	0.3487	0.1046	0.1144
398.1276	0.3707	0.1910	0.4049	0.7709
399.0613	0.6058	0.4117	0.6704	0.5437
425.0118	0.6627	0.4097	0.4013	0.9399
457.0669	0.3226	0.2481	0.3468	0.6961
480.7824	0.1071	0.0636	0.3287	0.1210
505.0207	0.5645	0.7728	0.4005	0.4565

Table S3 - Statistical analysis of the sulfates identified in plasma according to age groups. Significantly altered metabolites highlighted in red.

Sulfate	one-way ANOVA	Group I vs Group II	Group I vs Group III	Group II vs Group III
161.9844995	0.2939	0.1607	0.4555	0.2495
Phenol sulfate	0.9281	0.7604	0.8880	0.7862
Pyridin-2-yl sulfate	0.9402	0.4657	0.1892	0.5031
173.9923	0.9152	0.7530	0.9218	0.7465
p-Cresol sulfate	0.0492	0.6241	0.0259	0.0514
2-Aminophenol sulfate 1	0.4324	0.4194	0.2217	0.5423
2-Aminophenol sulfate 2	0.0295	0.7638	0.0398	0.0276
188.0088	0.0579	0.5931	0.0339	0.0752
Hydroquinone sulfate	0.0129	0.7873	0.0453	0.0109
Resorcinol sulfate	0.5427	0.3646	0.5151	0.5490
Cytosine sulfate	0.2413	0.5677	0.1318	0.2575
191.0179	0.1936	0.7053	0.2694	0.0727
4-Vinylphenol sulfate	0.5204	0.2843	0.3693	0.6979
4-Ethylphenylsulfate	0.3898	0.2639	0.6411	0.0868
2-Methoxyphenol sulfate	0.2107	0.3982	0.1052	0.3028
3-Hydroxy-5-methylphenyl sulfate	0.0483	0.1472	0.0382	0.1478
3-Methoxyphenol sulfate	0.1431	0.2076	0.0373	0.4467
5 methylcytosine sulfate	0.0851	0.2025	0.0274	0.2804
Pyrogallol sulfate 2	0.4980	0.3785	0.3120	0.9402
Pyrogallol sulfate 3	0.2793	0.4260	0.0982	0.4109
Pyrogallol sulfate 1	0.3193	0.2438	0.0844	0.7554
5,6-Dihydroxycyclohexa-1,3 dien-1 -yl sulfate	0.7462	0.7306	0.4249	0.6612
Indoxyl sulfate	0.2373	0.8889	0.1842	0.1921
Indoxyl sulfate 2	0.4273	0.3335	0.1761	0.7358
2,3-Dihydroxy-valeric acid sulfate	0.4747	0.6698	0.2371	0.4385

Chavicol sulfate	0.9737	0.7537	0.9093	0.9204
E)-4-(Prop-1-en-1-yl)phenyl sulfate	0.5103	0.3220	0.7604	0.1986
Tyramine sulfate	0.8162	0.6419	0.8708	0.6464
4-Hydroxybenzoic acid sulfate	0.0376	0.4264	0.0278	0.0761
2-(2-Hydroxyethyl)phenyl hydrogen sulfate	0.0785	0.5364	0.0669	0.0915
Creosol sulfate	0.8689	0.6479	0.6791	0.8448
218.8718	0.1828	0.7350	0.2100	0.0991
1-Methyl-pyrogallol-3-O-sulfate	0.6696	0.6676	0.4391	0.4400
2, 5 Dihydroxybenzyl alcohol sulfate	0.6311	0.4448	0.8209	0.4848
Benzene-1,2,3,5-tetrol sulfate	0.0931	0.5607	0.2255	0.0241
p-Butenylphenol sulfate	0.2998	0.1690	0.2116	0.8148
5,6-Dihydroxyindole sulfate 1	0.0974	0.3683	0.0683	0.1550
5,6-Dihydroxyindole sulfate 2	0.0857	0.5425	0.0737	0.1023
Thymol Sulfate	0.4098	0.3291	0.4513	0.2764
Acetamidophenol sulfate 2	0.1209	0.4149	0.3403	0.0269
Acetamidophenol sulfate 1	0.0643	0.9980	0.1172	0.0630
Paracetamol sulfate	0.2362	0.2294	0.2433	0.3072
230.0470	0.2056	0.4120	0.0261	0.3757
4-Hydroxyphenylacetic acid sulfate	0.1459	0.6668	0.1229	0.0876
Dopamine 4-sulfate	0.4301	0.2304	0.7083	0.2196
4-Hydroxy-3-(hydroxymethyl)benzyl sulfate	0.9894	0.9056	0.9130	0.9540
4-Phenylbutanoic acid O sulfate	0.1316	0.3422	0.0792	0.2187
3-[3-(Sulfooxy)phenyl]propanoic acid	0.4565	0.3072	0.4178	0.4755
2-Hydroxyacetaminophen sulfate	0.2366	0.2251	0.2488	0.2095
Methyltyramine sulfate	0.5731	0.3797	0.5454	0.5467
Hippuric acid sulfate	0.0824	0.6668	0.0722	0.1020
258.0425	0.2872	0.9086	0.3166	0.2226
Caffeic acid 3-sulfate	0.3302	0.9753	0.2881	0.2414
L-Tyrosine-O-sulfate	0.4744	0.2827	0.2280	0.9307

Homovanillic acid sulfate	0.3484	0.2521	0.4396	0.0464
Isoferulic acid sulfate	0.3107	0.7004	0.1132	0.3040
4-Hydroxyhippuric acid sulfate	0.3373	0.2203	0.1068	0.9364
274.0376989	0.2204	0.3833	0.1371	0.2916
3-Butylidene-7-hydroxyphthalide sulfate	0.5995	0.3762	0.3522	0.9808
5'-(3',4'-Dihydroxyphenyl)-gamma-valerolactone sulfate	0.2995	0.3270	0.9147	0.2198
305.0317	0.3538	0.3536	0.9921	0.2642
308.0763	0.1592	0.4356	0.0765	0.2315
352.0843	0.3592	0.4853	0.5248	0.1780
352.0844	0.3518	0.7074	0.3476	0.1246
356.1155	0.5096	0.4044	0.9108	0.3577
369.0808	0.4370	0.6490	0.5052	0.2085
372.1104	0.5904	0.3927	0.5645	0.5466
399.0609	0.9561	0.7928	0.8861	0.8572
425.0090	0.6107	0.3839	0.3176	0.9990
457.1488	0.7475	0.8623	0.5704	0.5087
480.7919	0.2539	0.0360	0.2795	0.6822

Table S4 – Pearson correlation between the metabolites and the variables age and gender in urine.

	Age		Gender	
	Pearson correlation	p-value	Pearson correlation	p-value
161.9859	-0.2086	0.2964	-0.3171	0.1312
Phenol sulfate	0.1101	0.5846	-0.1679	0.4330
Pyridin-2-yl sulfate	0.1040	0.6057	0.0435	0.8400
173.9939	0.0486	0.8096	-0.1181	0.5825
p-Cresol sulfate	0.2811	0.1555	-0.3295	0.1159
Aminophenol sulfate 2	0.2903	0.1419	-0.0187	0.9311
Aminophenol sulfate 1	0.2361	0.2357	-0.0435	0.8400
Aminophenol sulfate 3	0.2019	0.3126	0.0684	0.7509
188.0099	0.2997	0.1288	-0.4041	0.0502
Resorcinol sulfate	0.1428	0.4772	-0.1306	0.5432
Pyrocatechol sulfate	0.0474	0.8144	-0.0933	0.6647
Hydroquinone sulfate	0.3092	0.1165	0.0311	0.8854
189.003	0.0743	0.7126	-0.0684	0.7509
Cytosine sulfate	0.1566	0.4354	-0.0435	0.8400
6-Hydroxycyclohexa-1,3 dien-yl sulfate	0.0184	0.9276	0.2798	0.1855
4-Cyanophenyl sulfate	0.0520	0.7967	0.1430	0.5051
Vinylphenol sulfate 1	0.0049	0.9807	-0.2922	0.1659
Vinylphenol sulfate 2	-0.1743	0.3845	0.1430	0.5051
4-Ethylphenylsulfate	-0.1275	0.5261	-0.0062	0.9770
3-Hydroxy-5-methylphenyl sulfate	0.1630	0.4165	0.1803	0.3992
2-Methoxyphenol sulfate	0.2217	0.2663	-0.1803	0.3992
3-Methoxyphenol sulfate	0.3413	0.0814	-0.3419	0.1020
203.9724	0.1015	0.6143	0.0933	0.6647
Aminohydroxyphenyl sulfate	0.6380	0.0003	-0.2798	0.1855

5-Methylcytosine sulfate	0.3138	0.1109	-0.3668	0.0779
Pyrogallol sulfate 4	0.2104	0.2921	-0.1430	0.5051
Pyrogallol sulfate 1	0.5545	0.0027	-0.1430	0.5051
Pyrogallol sulfate 3	-0.1581	0.4308	0.1679	0.4330
5,6-Dihydroxycyclohexa-1,3 dien-1 -yl sulfate	-0.1422	0.4792	-0.0062	0.9770
Indoxyl 3 sulfate	0.0850	0.6733	-0.1803	0.3992
2,3-Dihydroxy-valeric acid sulfate	0.1107	0.5825	-0.3419	0.1020
Chavicol sulfate	0.0232	0.9084	-0.1927	0.3669
E-4-(Prop-1-en-1-yl)phenyl sulfate	0.0113	0.9553	-0.1927	0.3669
Vinylbenzene diol sulfate	0.0168	0.9336	0.2300	0.2796
2-Acetylphenyl sulfate	0.0569	0.7781	0.0311	0.8854
Tyramine sulfate	0.0817	0.6855	-0.5036	0.0121
Hydroxybenzoic acid sulfate 3	0.2982	0.1308	-0.2300	0.2796
Hydroxybenzoic acid sulfate 2	0.3615	0.0639	-0.1554	0.4684
Creosol sulfate	-0.0043	0.9831	0.0684	0.7509
2-(2-Hydroxyethyl)phenyl hydrogen sulfate	0.0651	0.7468	-0.1927	0.3669
218.873	-0.0489	0.8085	-0.1927	0.3669
218.905	0.0437	0.8285	-0.2798	0.1855
218.9968	0.1055	0.6004	0.2176	0.3071
218.9959	0.0401	0.8427	0.1927	0.3669
218.996	0.1052	0.6015	0.1554	0.4684
1-Methyl-pyrogallol-3-O-sulfate	-0.0321	0.8737	0.0311	0.8854
2, 5 Dihydroxybenzyl alcohol sulfate	-0.1936	0.3332	0.1554	0.4684
Benzene-1,2,3,5-tetrol sulfate	0.1278	0.5251	0.2425	0.2537
227.0215	0.1245	0.5362	0.1306	0.5432
p-Butenylphenol sulfate	-0.0144	0.9433	0.0062	0.9770
5,6-Dihydroxyindole sulfate 1	0.5169	0.0058	-0.2798	0.1855
5,6-Dihydroxyindole sulfate 2	0.5738	0.0018	-0.1927	0.3669
Methoxy-vinylphenol sulfate	0.1340	0.5053	-0.1554	0.4684

Thymol sulfate	-0.0667	0.7411	-0.2922	0.1659
229.9958	0.4089	0.0342	-0.2549	0.2294
Paracetamol sulfate	0.1015	0.6143	-0.4165	0.0429
Acetamidophenol sulfate 2	0.0875	0.6644	0.1057	0.6231
Acetamidophenol sulfate 1	0.1563	0.4363	-0.0808	0.7074
230.0487	0.3970	0.0403	-0.2549	0.2294
2,4 dihydroxy acetophenone sulfate 1	0.1646	0.4121	-0.3171	0.1312
4-Hydroxyphenylacetic acid sulfate	0.0462	0.8191	-0.3295	0.1159
2,4 dihydroxy acetophenone sulfate 2	-0.0018	0.9928	0.1430	0.5051
2-(4-Methoxyphenyl)ethyl hydrogen sulfate	0.0483	0.8108	0.0808	0.7074
(4-Ethyl-2-methoxyphenyl)oxidanesulfonic acid	-0.1220	0.5443	-0.1181	0.5825
Dopamine-4-sulfate	0.1306	0.5161	-0.1430	0.5051
Dopamine-3-sulfate	0.1750	0.3828	-0.2922	0.1659
Hydroxytyrosol sulfafte	-0.0765	0.7046	0.0808	0.7074
4-Hydroxy-3-(hydroxymethyl)benzyl sulfate	-0.0933	0.6435	-0.3792	0.0676
Methoxybenzene triol sulfate 1	-0.0915	0.6501	-0.0560	0.7951
Methoxybenzene triol sulfate 2	0.1006	0.6175	-0.1679	0.4330
238.0173	0.1575	0.4326	-0.5036	0.0121
239.8787	0.3374	0.0853	-0.2798	0.1855
Quinoline-4,8-diol sulfate	0.0012	0.9952	-0.3544	0.0893
240.9807	0.2909	0.1410	-0.2176	0.3071
241.9756	0.0171	0.9324	-0.2300	0.2796
241.9757	-0.1413	0.4820	-0.2052	0.3362
242.012	0.1838	0.3587	-0.1679	0.4330
trans-3-Hydroxycinnamic acid sulfate	-0.0645	0.7491	-0.1927	0.3669
trans-4-Hydroxycinnamic acid sulfate	0.0018	0.9928	-0.0684	0.7509
4-Phenylbutanic acid O sulfate 1	0.1774	0.3760	-0.0311	0.8854
243.991	0.4022	0.0375	-0.3295	0.1159
Phloretic acid sulfate 1	-0.0587	0.7711	0.1057	0.6231

Phloretic acid sulfate 2	0.2554	0.1985	-0.1181	0.5825
2-tert-Butylhydroquinone sulfate	-0.1517	0.4500	-0.1306	0.5432
2-Hydroxyacetaminophen sulfate	0.1453	0.4697	-0.3544	0.0893
246.0433	0.3245	0.0986	-0.3668	0.0779
246.0432	0.0147	0.9421	-0.2052	0.3362
Dihydroxyphenylacetic acid sulfate	0.2221	0.2656	-0.4290	0.0365
Vanillic acid sulfate	-0.1025	0.6111	-0.0933	0.6647
Homovanillyl alcohol sulfate	0.0587	0.7711	0.0435	0.8400
256.028	0.0272	0.8928	-0.0808	0.7074
5-hydroxytryptophol sulfate	0.1961	0.3270	-0.1430	0.5051
256.9754	0.1667	0.4060	-0.2673	0.2067
Hippuric acid sulfate	0.1138	0.5720	-0.1554	0.4684
258.0437	-0.1441	0.4734	-0.0933	0.6647
Caffeic acid sulfate 1	0.2747	0.1656	-0.1679	0.4330
Caffeic acid sulfate 2	-0.3340	0.0886	-0.2300	0.2796
Propylparaben sulfate	-0.0976	0.6283	-0.3668	0.0779
L-Tyrosine-O-sulfate	-0.0070	0.9722	-0.3295	0.1159
3,4 Dihydrocinnamic acid sulfate	0.1208	0.5483	-0.4911	0.0148
Homovanillic acid sulfate 1	0.1101	0.5846	-0.0684	0.7509
Homovanillic acid sulfate 2	0.0269	0.8940	-0.0684	0.7509
Dihydroxyconiferyl alcohol sulfate	-0.1921	0.3371	-0.0560	0.7951
267.9578	0.0850	0.6733	-0.0684	0.7509
268.9425	0.3114	0.1139	-0.2176	0.3071
[(6-Hydroxy-1-oxo-1H-isochromen-3-yl)methoxy]sulfonic acid	-0.1447	0.4715	0.0435	0.8400
Isoferulic acid sulfate	-0.1881	0.3474	-0.1181	0.5825
4-Hydroxyhippuric acid sulfate	0.4154	0.0312	0.2425	0.2537
274.0385	0.0725	0.7194	-0.0062	0.9770
281.0603	-0.3153	0.1091	-0.1181	0.5825

281.0699	-0.1661	0.4077	-0.1927	0.3669
3-Butylidene-7-hydroxyphthalide sulfate	-0.0349	0.8629	0.0808	0.7074
5'-(3',4'-Dihydroxyphenyl)-gamma-valerolactone sulfate 1	-0.0125	0.9505	-0.3046	0.1478
5'-(3',4'-Dihydroxyphenyl)-gamma-valerolactone sulfate 2	-0.1670	0.4051	-0.1181	0.5825
288.9517	0.0749	0.7103	-0.2922	0.1659
4-Hydroxy-5-(3'-hydroxyphenyl)-valeric acid-3'-O-sulphate	-0.0566	0.7792	-0.0187	0.9311
291.9577	0.0835	0.6788	-0.1181	0.5825
293.9563	-0.0459	0.8202	-0.1181	0.5825
Methyl dioxindole-3-acetate sulfate	0.1820	0.3636	0.0062	0.9770
N-Acetylgalactosamine 6-sulfate	-0.4692	0.0136	0.2052	0.3362
Sinapic acid sulfate	-0.1441	0.4734	-0.2300	0.2796
305.0331	-0.0569	0.7781	-0.0560	0.7951
307.9529	0.4193	0.0295	-0.3295	0.1159
307.9896	0.0801	0.6911	-0.3668	0.0779
308.0771	0.1031	0.6089	-0.1430	0.5051
309.0981	0.0456	0.8214	-0.2176	0.3071
311.9852	0.0202	0.9204	-0.2425	0.2537
318.065	0.0514	0.7991	-0.0684	0.7509
325.0399	-0.1150	0.5679	-0.0435	0.8400
326.9476	-0.1370	0.4955	0.0435	0.8400
N-acryloyl-3,4-dihydroxy-DL-phenylalanine sulfate	0.0101	0.9601	-0.0933	0.6647
3-(2-((3,4-Dihydroxybenzyl)amino)ethyl)phenyl sulfate 1	-0.2193	0.2717	-0.0560	0.7951
3-(2-((3,4-Dihydroxybenzyl)amino)ethyl)phenyl sulfate 2	-0.2361	0.2357	0.0062	0.9770
338.0809	0.0544	0.7874	0.2176	0.3071
340.9641	-0.0651	0.7468	-0.0933	0.6647
341.0509	0.0018	0.9928	-0.0187	0.9311
342.1014	-0.2104	0.2921	0.2176	0.3071
344.1168	-0.1269	0.5281	0.1306	0.5432
347.1687	0.2239	0.2616	-0.5782	0.0031

352.0863	-0.2584	0.1930	-0.0808	0.7074
352.0868	-0.2416	0.2247	-0.1679	0.4330
353.9948	0.0251	0.9012	-0.1306	0.5432
356.1171	0.0125	0.9505	0.0684	0.7509
357.1203	-0.0031	0.9879	0.0808	0.7074
Nigellic acid sulfate	0.1037	0.6068	-0.1430	0.5051
369.0817	-0.1003	0.6186	-0.0187	0.9311
370.0964	0.0128	0.9493	-0.1803	0.3992
372.1118	0.1346	0.5033	0.0933	0.6647
372.1125	0.0667	0.7411	-0.0062	0.9770
Enterolactone sulfate	0.3527	0.0712	-0.0435	0.8400
378.1018	-0.1823	0.3628	-0.0933	0.6647
Pyrogallol-2-O-glucuronide sulfate	-0.0713	0.7239	0.0684	0.7509
381.1021	0.2979	0.1312	-0.2052	0.3362
388.0506	0.0046	0.9819	0.0435	0.8400
393.0514	0.3392	0.0835	-0.0684	0.7509
398.1276	-0.1040	0.6057	-0.2425	0.2537
399.0613	0.2153	0.2808	-0.0311	0.8854
425.0118	0.1743	0.3845	-0.0933	0.6647
457.0669	-0.1734	0.3870	-0.0435	0.8400
480.7824	-0.0997	0.6207	-0.1057	0.6231
505.0207	0.1618	0.4201	-0.3792	0.0676

Table S5 – Pearson correlation between the metabolites and the variables age and gender in plasma.

	Age		Gender	
	Pearson correlation	p-value	Pearson correlation	p-value
161.9845	-0.0104	0.958937	-0.49112	0.014809
Phenol sulfate	0.046498	0.817859	0.180284	0.399229
Pyridin-2-yl sulfate	0.257266	0.195157	0.230018	0.279573
173.9923	0.049557	0.806093	0.155417	0.46835
p-Cresol sulfate	0.483556	0.010608	-0.05596	0.795075
2-Aminophenol sulfate 1	0.234017	0.240054	0.080817	0.707363
2-Aminophenol sulfate 2	0.393087	0.042522	0.304618	0.14781
188.0088	0.442338	0.02087	-0.04352	0.839993
Hydroquinone sulfate	0.455186	0.017045	0.230018	0.279573
Resorcinol sulfate	0.315082	0.109416	-0.11812	0.582529
Cytosine sulfate	0.321506	0.101988	0.031083	0.885356
191.0179	0.253289	0.202394	0.068384	0.750866
4-Vinylphenol sulfate	0.146834	0.464873	-0.08082	0.707363
4-Ethylphenylsulfate	0.18079	0.36683	-0.06838	0.750866
2-Methoxyphenol sulfate	0.390334	0.044123	0.01865	0.931072
3-Hydroxy-5-methylphenyl sulfate	0.372592	0.05562	0.167851	0.433048
3-Methoxyphenol sulfate	0.474458	0.012403	-0.29218	0.165916
5 methylcytosine sulfate	0.501072	0.007759	-0.18028	0.399229
Pyrogallol sulfate 2	-0.16213	0.419118	0.267318	0.206658
Pyrogallol sulfate 3	0.302234	0.125466	0.130551	0.543165
Pyrogallol sulfate 1	0.678191	0.000101	-0.05595	0.795118
5,6-Dihydroxycyclohexa-1,3 dien-1 -yl sulfate	-0.17131	0.392907	0.167851	0.433048
Indoxyl sulfate	0.218416	0.273735	0.105684	0.623084
Indoxyl sulfate 2	0.259407	0.191335	0.118117	0.582529

2,3-Dihydroxy-valeric acid sulfate	0.211992	0.288443	0.05595	0.795118
Chavicol sulfate	-0.01315	0.94808	-0.03108	0.885356
E)-4-(Prop-1-en-1-yl)phenyl sulfate	0.224228	0.260851	-0.06838	0.750866
Tyramine sulfate	0.065158	0.746777	-0.13055	0.543165
4-Hydroxybenzoic acid sulfate	0.474458	0.012403	-0.03108	0.885356
2-(2-Hydroxyethyl)phenyl hydrogen sulfate	0.561947	0.002285	-0.06838	0.750866
Creosol sulfate	0.110737	0.582404	0.130551	0.543165
218.8718	0.447844	0.019152	-0.13055	0.543165
1-Methyl-pyrogallol-3-O-sulfate	0.132763	0.509162	0.317052	0.131153
2, 5 Dihydroxybenzyl alcohol sulfate	0.014683	0.942052	0.230018	0.279573
Benzene-1,2,3,5-tetrol sulfate	0.284185	0.150828	0.404085	0.050187
p-Butenylphenol sulfate	-0.0312	0.877218	-0.11812	0.582529
5,6-Dihydroxyindole sulfate 1	0.479964	0.011289	-0.15542	0.46835
5,6-Dihydroxyindole sulfate 2	0.481494	0.010995	-0.04352	0.839993
Thymol Sulfate	0.082594	0.682125	-0.60302	0.001814
Acetamidophenol sulfate 2	0.324871	0.09825	0.391652	0.058401
Acetamidophenol sulfate 1	0.275314	0.164555	-0.00622	0.977
Paracetamol sulfate - Prepared	0.309576	0.116097	-0.19272	0.366941
230.047	0.5595	0.002411	-0.09325	0.664731
4-Hydroxyphenylacetic acid sulfate	0.413277	0.032139	-0.29218	0.165916
Dopamine 4-sulfate	0.305293	0.121497	-0.04352	0.839993
4-Hydroxy-3-(hydroxymethyl)benzyl sulfate	0.218722	0.273047	-0.06838	0.750866
4-Phenylbutanoic acid O sulfate	0.439891	0.021672	0.043517	0.839993
3-[3-(Sulfooxy)phenyl]propanoic acid	0.317223	0.106897	0.09325	0.664731
2-Hydroxyacetaminophen sulfate	0.341084	0.081665	-0.05595	0.795118
Methyltyramine sulfate	0.152341	0.448109	-0.18028	0.399229
Hippuric acid sulfate	0.336189	0.086429	-0.03108	0.885356
258.0425	-0.0104	0.958937	-0.00622	0.977
Caffeic acid 3-sulfate	0.096666	0.631477	0.01865	0.931072

L-Tyrosine-O-sulfate	0.319976	0.103721	-0.11812	0.582529
Homovanillic acid sulfate	0.359132	0.065808	-0.06838	0.750866
Isoferulic acid sulfate	0.348731	0.074625	0.155417	0.46835
4-Hydroxyhippuric acid sulfate	0.433773	0.02379	0.155417	0.46835
274.0377	0.441115	0.021268	-0.05595	0.795118
3-Butylidene-7-hydroxyphthalide sulfate	0.201897	0.312545	0.105684	0.623084
5'-(3',4'-Dihydroxyphenyl)-gamma-valerolactone sulfate	0.062099	0.758309	-0.03108	0.885356
305.0317	0.072805	0.718185	-0.05595	0.795118
308.0763	0.382381	0.049019	0.130551	0.543165
352.0843	-0.01927	0.923989	0.01865	0.931072
352.0844	-0.07954	0.693325	0.192718	0.366941
356.1155	0.046192	0.819038	0.242451	0.253666
369.0808	0.129704	0.519056	0.205151	0.336221
372.1104	0.133069	0.508177	0.167851	0.433048
399.061	0.025696	0.898764	0.118117	0.582529
425.009	0.167024	0.405021	0.130551	0.543165
457.1488	0.215357	0.280678	-0.39165	0.058401
480.7919	-0.13827	0.491589	-0.31705	0.131153