

**Supplementary Table 4** Identified metabolites in urine, serum and faeces by untargeted metabolomics

#	Tentative annotation	Sample	Level of identification <sub>1</sub>	MS mode	Adduct	rt* (min)	Experimental m/z	Authentic standard m/z	Database m/z	Mass error (mDa)
1	Allantoic acid	Serum	1	ESI+	[M+H]	0.46	177.0608	177.0630		2.2
2	Trimethylamine N-oxide	Serum; Urine	1	ESI+	[M+H]	0.50	76.0759	76.0759		0.0
3	Carnitine	Serum; Urine	1	ESI+	[M+H]	0.52	162.1124	162.1134		1.0
4	Betaine	Serum	1	ESI+	[M+H]	0.52	118.0865	118.0867		0.2
5	Citrulline	Faeces; Serum	1	ESI-	[M-H]	0.54	174.0872	174.0879		0.7
6	2-aminoisobutyric acid	Faeces	1	ESI-	[M-H]	0.54	102.0546	102.0554		0.6
7	Imidazolelactic acid	Urine	3	ESI-	[M-H]	0.54	155.0458	-	155.0462	0.4
8	Imidazolepropionic acid	Urine	1	ESI+	[M+H]	0.56	141.0670	141.0658		1.2
9	Proline	Faeces; Serum	1	ESI+	[M+H]	0.56	116.0707	116.0711		0.4
10	Proline betaine	Serum; Urine	1	ESI+	[M+H]	0.58	144.1023	144.1019		0.4
11	Propionylcholine / Meta-choline	Urine	3	ESI+	[M+H]	0.62	160.1337	-	160.1332	0.5
12	Dopamine	Faeces	1	ESI+	[M+H]	0.62	154.0847	154.0853		0.6
13	Nicotinamide	Faeces	1	ESI+	[M+H]	0.62	123.0561	123.0566		0.5
14	Citric acid	Serum; Urine	1	ESI-	[M-H]	0.64	191.0190	191.0192		0.2
15	Valine	Faeces; Serum	1	ESI+	[M+H-HCOOH]	0.66	72.0810	72.0814		0.4
16	Acetylcarnitine	Serum; Urine	1	ESI+	[M+H]	0.67	204.1240	204.1240		0.0
				ESI+	[M+H] fragment	0.67	145.0507	145.0510		0.3
				ESI+	[M+H] fragment	0.67	85.0289	85.0290		0.1
				ESI+	[M+H] fragment	0.68	60.0809	60.0830		2.1

17	Pipecolic acid betaine	Serum	1	ESI+	[M+H]	0.71	158.1170	158.1174	0.4	
18	N-Acetylcadaverine	Faeces	3	ESI+	[M+H]	0.73	145.1325	-	145.1335	1.0
19	Hypoxanthine	Faeces; Serum	1	ESI+	[M+H]	0.76	137.0462	137.0468	0.6	
20	Hydroxybutyrylcarnitine	Urine	3	ESI+	[M+H]	0.77	248.1505	-	248.1492	1.3
21	Uridine	Faeces; Serum	1	ESI-	[M-H]	0.83	243.0616	243.0606	1.0	
22	N-Acetylglutamic acid	Serum	1	ESI+	[M+H-C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> ]	0.79	130.0502	130.0497	0.5	
23	Succinylcarnitine / Methylmalonylcarnitine	Faeces	3	ESI+	[M+H]	0.79	262.1285		262.1285	0.0
24	Tyrosine	Faeces; Serum; Urine	1	ESI+	[M+H]	0.82	182.0816	182.0819	0.3	
				ESI-	[M-H]	0.82	180.0647	180.0666	1.9	
25	3-Methylthiohexyl acetate / 3-Mercaptoheptyl acetate	Urine	3	ESI-	[M-H]	0.83	189.0962		189.0955	0.7
26	Methylcysteine sulfoxide	Urine	3	ESI-	[M+Cl]	0.88	185.9978		185.9997	1.9
27	1-(1-Pyrrolidinyl)-2-butanone	Urine	3	ESI+	[M+H]	0.89	142.1235		142.1226	0.9
				ESI+	[M+NH <sub>4</sub> ]	0.89	159.1500		159.1492	0.8
28	Methoxy-Pyrogallol	Urine	3	ESI-	[M-H]	0.93	139.0400		139.0401	0.1
29	Isoleucine	Faeces; Serum; Urine	1	ESI+	[M+H]	0.94	132.1029	132.1024	0.5	
				ESI+	[M+H] fragment	0.94	86.0969	86.0972	0.3	
30	Inosine	Serum	1	ESI-	[M-H]	0.94	267.0720	267.0730	1.0	
31	Dihydroxybenzoic acid-glucuronide	Urine	3	ESI-	[M-H]	1.01	329.0492		329.0514	2.2
	Leucine	Faeces; Serum; Urine	1	ESI-	[M-H]	1.06	130.0863	130.0868	0.5	

				ESI+	[M+H] fragment	1.03	86.0967	86.0972	0.5
<b>32</b>	Propionylcarnitine	Urine	1	ESI+	[M+H]	1.02	218.1396	218.1400	0.4
				ESI+	[M+H] fragment	1.02	159.0658	159.0660	0.2
				ESI+	[M+H] fragment	1.02	85.0288	85.0290	0.2
<b>33</b>	5-hydroxytryptophan	Urine	1	ESI+	[M+H-HCOOH]	1.11	175.0875	175.0876	0.1
			1	ESI-	[M-H]	1.13	219.0769	219.0759	1.0
<b>34</b>	3-Hydroxyisovaleryl carnitine	Urine	3	ESI+	[M+H]	1.13	262.1661	262.1649	1.2
<b>35</b>	2-hydroxybutyric acid	Urine	1	ESI-	[M-H]	1.17	103.0395	103.0400	0.5
<b>36</b>	Ophthalmic acid	Urine	3	ESI-	[M-H]	1.28	288.1186	288.1201	1.5
				ESI-	[M-H-H <sub>2</sub> O]	1.28	270.1087	270.1090	0.3
				ESI-	[M-H] fragment	1.28	253.0822	-	-
<b>37</b>	Casimiroedine	Serum	3	ESI+	[M+H]	1.29	418.1933	418.1973	4.0
<b>38</b>	Pyrogallol-sulphate-glucuronide	Urine	3	ESI-	[M-H]	1.43	381.0119	381.0133	1.4
				ESI-	[M-H-glucuronide]	1.42	204.9812	204.9812	0.0
<b>39</b>	Kynurenine	Urine	1	ESI+	[M+H-NH <sub>3</sub> -COCH <sub>2</sub> ]	1.45	150.0557	150.0542	1.5
<b>40</b>	Gammaglutamylvaline	Urine	1	ESI+	[M+H]	1.47	247.1289	247.1300	1.1
				ESI+	[M+H] fragment	1.48	230.1032	230.1030	0.2
				ESI+	[M+H] fragment	1.48	184.0973	184.0980	0.7
				ESI+	[M+H] fragment	1.47	118.0869	118.0870	0.1
				ESI+	[M+H] fragment	1.48	72.0810	72.0810	0.0
<b>41</b>	Pyrogallol-sulphate	Urine	3	ESI-	[M-H]	1.50	204.9807	204.9812	0.5

42	Dihydroxybenzoic acid-glycine	Urine	3	ESI-	[M-H]	1.60	210.0406	210.0408	0.2
43	Phenylalanine	Faeces; Serum; Urine	1	ESI+	[M+H-HCOOH]	1.61	120.0815	120.0815	0.0
				ESI-	[M-H]	1.62	164.0702	164.0700	0.2
				ESI+	[M+H]	1.63	166.0860	168.0854	0.6
44	3-Hydroxyisovaleric acid	Urine	1	ESI-	[M-H]	1.66	117.0551	117.0560	0.9
45	Methoxy-Pyrogallol-sulphate	Urine	3	ESI-	[M-H]	1.91	218.9963	218.9969	0.6
				ESI-	[M-H-CH <sub>2</sub> ]	1.91	204.9807	204.9812	0.5
				ESI-	[M-H-sulfate]	1.91	139.0397	139.0401	0.4
46	Isobutyryl-L-carnitine	Urine	3	ESI+	[M+H]	1.96	232.1552	232.1543	0.9
				ESI+	[M+H] fragment	1.96	173.0812	-	-
				ESI+	[M+H] fragment	1.96	85.0289	-	-
				ESI+	[M+H] fragment	1.96	60.0809	-	-
47	3-(3,5-dihydroxyphenyl)propanoic acid-glucuronide	Urine	3	ESI-	[M-H]	1.98	357.0810	357.0827	1.7
				ESI+	[M+H-glucuronide]	1.98	183.0654	183.0652	0.2
				ESI+	[M+H-H <sub>2</sub> O-glucuronide]	1.98	165.0559	165.0546	1.3
48	3,5-dihydroxybenzoic acid	Urine	1	ESI-	[M-H]	1.99	153.0192	153.0181	1.1
49	Pantothenic acid	Urine	1	ESI+	[M+H]	2.01	220.1187	220.1187	0.0
				ESI-	[M-H]	2.02	218.1028	218.1031	0.3
50	Theobromine	Serum	1	ESI+	[M+H]	2.06	181.0717	181.0707	1.0
				ESI+	[M+H-H <sub>2</sub> O]	2.06	163.0608	163.0618	1.0

<b>51</b>	3-hydroxyanthranilic acid	Urine	1	ESI+	[M+H-H <sub>2</sub> O]	2.11	136.0405	136.0392	1.3
<b>52</b>	3-(3,5-dihydroxyphenyl)propanoic acid-sulphate	Urine	3	ESI-	[M-H]	2.17	261.0068	261.0074	0.6
ESI-				[M-H-sulfate]	2.18	181.0501	181.0506	0.5	
ESI-				[M-H-CO <sub>2</sub> -sulfate]	2.18	137.0616	137.0608	0.8	
<b>53</b>	Tryptophan	Faeces; Serum; Urine	1	ESI+	[M+H]	2.40	205.0979	205.0981	0.2
ESI-				[M-H]	2.40	203.0822	203.0821	0.1	
<b>54</b>	1,7-dimethylxanthine	Serum	3	ESI+	[M+H]	2.53	181.0718	181.0720	-
ESI+				[M+H] fragment	2.53	124.0508	-	-	
<b>55</b>	5,6-Dihydroxyindole	Urine	3	ESI+	[M+H]	2.53	150.0556	150.0550	0.6
ESI+				[M+H-H <sub>2</sub> O]	2.53	132.0454	132.0444	1.0	
<b>56</b>	Phenol sulfate	Urine	1	ESI-	[M-H]	2.57	172.9907	172.9902	0.5
ESI-				[M-H-sulfate]	2.57	93.0338	-	-	
ESI-				[M-H-phenol]	2.58	79.9564	-	-	
<b>57</b>	Xanthurenic acid	Urine	1	ESI-	[M-H]	2.57	204.0295	204.0302	0.7
ESI+				[M+H]	2.58	206.0456	206.0460	0.4	
ESI+				[M+H-H <sub>2</sub> O]	2.58	188.0345	188.0352	0.7	
ESI+				[M+H-HCOOH]	2.58	160.0400	160.0405	0.5	
<b>58</b>	Caffeic acid-sulfate	Urine	3	ESI-	[M-H]	2.60	258.9911	258.9918	0.7
<b>59</b>	Caffeic acid-sulfate	Urine	3	ESI-	[M-H]	2.65	258.9913	258.9918	0.5
<b>60</b>	3,5-dihydroxyhydrocinnamic acid	Urine	3	ESI+	[M+H-HCOOH]	2.66	137.0606	137.0597	0.9

<b>61</b>	Tryptamine	Urine	1	ESI+	[M+H-NH3]	2.66	144.0815	144.0820	0.5
<b>62</b>	Tiglylcarnitine	Urine	3	ESI+	[M+H]	2.69	244.1551	244.1543	0.8
				ESI+	[M+H] fragment	2.69	185.0813	-	-
				ESI+	[M+H] fragment	2.68	181.0615	-	-
				ESI+	[M+H] fragment	2.68	135.1373	-	-
				ESI+	[M+H] fragment	2.68	135.0562	-	-
				ESI+	[M+H] fragment	2.68	106.0293	-	-
				ESI+	[M+H] fragment	2.69	85.0289	-	-
				ESI+	[M+H] fragment	2.68	78.0344	-	-
<b>63</b>	Indoxyl sulfate	Serum	1	ESI-	[M-H]	2.70	212.0008	212.0037	2.9
<b>64</b>	Isovalerylglycine	Urine	1	ESI-	[M-H]	2.71	158.0817	158.0807	1.0
<b>65</b>	Dihydroferulic acid 4-O-glucuronide	Urine	3	ESI-	[M-H]	2.71	371.0974	371.0984	1.0
<b>66</b>	Methylpyrogallol-sulfate	Urine	3	ESI-	[M-H]	2.72	218.9965	218.9969	0.4
				ESI-	[M-H-sulfate]	2.72	139.0397	139.0401	0.4
<b>67</b>	Dihydroxycinnamic acid-sulfate	Urine	3	ESI-	[M-H]	2.75	258.9914	258.9918	0.6
				ESI-	[M-H-sulfate]	2.75	179.0348	179.0350	0.2
<b>68</b>	3-methylpyrogallol-sulfate	Urine	1	ESI-	[M-H]	2.77	218.9965	218.9941	2.4
				ESI-	[M-H-sulfate]	2.77	139.0399	139.0401	0.2
<b>69</b>	Tryptophan betaine	Serum; Urine	1	ESI+	[M+H]	2.78	247.1444	247.1450	0.6
				ESI+	[M+H-C3H9N]	2.78	188.0705	188.0707	0.2
				ESI+	[M+H] fragment	2.78	146.0602	-	-
				ESI+	[M+H] fragment	2.78	60.0810	-	-

				ESI-	[M-H] fragment	2.83	142.0655	-	-
<b>70</b>	5-Hydroxyindole-3-acetic acid	Urine	1	ESI-	[M-H-HCOOH]	2.78	144.0449	144.0454	0.5
<b>71</b>	Dihydroxycinnamic acid-sulfate	Urine	3	ESI-	[M-H]	2.82	258.9909	258.9918	0.9
				ESI-	[M-H-sulfate]	2.82	179.0342	179.0350	0.8
<b>72</b>	Isovalerylcarnitine	Urine	1	ESI+	[M+H]	2.85	246.1710	246.1709	0.1
				ESI+	[M-H] fragment	2.85	187.0973	-	-
				ESI+	[M-H] fragment	2.85	85.0289	-	-
<b>73</b>	2-Methylbutyroylcarnitine / Pivaloylcarnitine / Valerylcarnitine	Urine	3	ESI+	[M+H]	2.90	246.1709	246.1700	0.9
				ESI+	[M-H] fragment	2.90	187.0973	-	-
				ESI+	[M-H] fragment	2.89	85.0288	-	-
<b>74</b>	Dihydroferuloylglycine / N-Acetylvani alanine	Urine	3	ESI-	[M-H]	2.92	252.0870	252.0877	0.7
<b>75</b>	Dihydroxycinnamic acid-sulfate	Urine	3	ESI-	[M-H]	2.95	258.9911	258.9918	0.7
				ESI-	[M-H-sulfate]	2.95	179.0343	179.0350	0.7
<b>76</b>	Dihydroxycinnamic acid	Faeces	3	ESI-	[M-H]	2.99	181.0502	181.0506	0.4
<b>77</b>	Dihydroxycinnamic acid-sulfate	Urine	3	ESI-	[M-H]	3.00	258.9913	258.9918	0.5
				ESI-	[M-H-sulfate]	3.00	179.0342	179.0350	0.8
<b>78</b>	Dihydrocaffeic acid-sulfate	Urine	3	ESI-	[M-H]	3.02	261.0044	261.0074	3.0
				ESI-	[M-H-sulfate]	3.02	181.0493	181.0506	1.3

<b>79</b>	2,4-dihydroxycinnamic acid	Faeces	3	ESI-	[M-H]	3.06	181.0497	181.0506	0.9
<b>80</b>	Hippuric acid	Serum; Urine	1	ESI-	[M-H]	3.06	178.0503	178.0504	0.1
				ESI+	[M+H]	3.07	180.0660	180.0660	0.0
<b>81</b>	Caffeine	Serum	1	ESI+	[M+H]	3.12	195.0876	195.0882	0.6
<b>82</b>	N-lactoyl-Valine / Hydroxyhexanoylglycine	Urine	3	ESI-	[M-H]	3.12	188.0923	188.0928	0.5
<b>83</b>	Phenylacetylglutamine	Urine	1	ESI-	[M-H]	3.15	263.1030	263.1020	1.0
				ESI+	[M+H-H2O]	3.16	247.1084	-	-
<b>84</b>	Benzeneacetamide-sulphate	Urine	3	ESI-	[M-H]	3.30	230.0120	230.0129	0.9
				ESI-	[M-H-sulfate]	3.30	150.0557	150.0561	0.4
<b>85</b>	Indole-3-carboxylic acid-glucuronide	Urine	1	ESI-	[M-H]	3.40	336.0712	336.0704	0.8
				ESI-	[M-H] fragment	3.40	193.0351	193.0341	1.0
<b>86</b>	P-cresol sulfate	Urine; Serum	1	ESI-	[M-H]	3.44	187.0051	187.0053	0.2
				ESI-	[M-H-SO3]	3.44	107.0495	107.0505	1.0
				ESI-	[M-H-cresol]	3.44	79.9563	79.9589	3.6
				ESI-	[2M-H]	3.44	375.0201	375.0194	0.7
				ESI-	[2M-2H+Na]	3.44	397.0048	397.0044	0.4
<b>87</b>	Oxindole-3-acetic acid	Faeces; Urine	1	ESI-	[M-H]	3.42	190.0502	190.0480	2.2
				ESI-	[M-H-CO2]	3.42	146.0609	146.0590	1.9
				ESI+	[M+H-CO2]	3.42	146.0610	-	-
<b>88</b>	Urolithin C-glucuronide	Urine	1	ESI-	[M-H-glucuronide]	3.42	243.0313	243.0294	1.9
<b>89</b>	O-methoxycatechol-O-sulphate	Urine	3	ESI-	[M-H]	3.44	203.0014	203.0020	0.6

<b>90</b>	Urolithin A-glucuronide	Urine	1	ESI+	[M+H]	3.45	405.0826	405.0870	4.4
				ESI+	[M+H-glucuronide]	3.44	229.0507	229.0520	1.3
				ESI-	[M-H-glucuronide]	3.46	227.0341	-	-
<b>91</b>	Kiwiionoside	Urine	3	ESI-	[M-H]	3.44	405.2123	405.2130	0.7
<b>92</b>	Indole-3-acetic acid-glucuronide	Urine	1	ESI-	[M-H]	3.46	350.0868	350.0861	0.7
				ESI-	[M-H-NH3-CO-COCH2-C4H6O]	3.46	193.0351	193.0334	0.7
				ESI-	[M-H] fragment	3.46	174.0553	-	-
				ESI+	[M+NH4]	3.45	369.1286	-	-
				ESI+	[M+H-glucuronide]	3.45	176.0709	-	-
<b>93</b>	3-hydroxyoctanoyl carnitine	Urine	3	ESI+	[M+H]	3.47	304.2127	304.2119	0.8
<b>94</b>	Phenylalanylphenylalanine	Serum	3	ESI+	[M+H]	3.47	313.1550	313.1547	0.3
				ESI+	[M+H-phenylalanine]	3.47	166.0860	166.0863	0.3
				ESI+	[M+H] fragment (C8H9N)	3.47	120.0810	120.0808	0.2
<b>95</b>	Methylhippuric acid	Urine	1	ESI-	[M-H]	3.48	192.0662	192.0657	0.5
				ESI-	[M-H-CO2]	3.49	148.0764	148.0767	0.3
<b>96</b>	3-hydroxydecanoyl carnitine	Urine	3	ESI+	[M+H]	3.49	332.2431	332.2431	0.0
				ESI+	[M+H] fragment	3.49	302.1982	-	-
<b>97</b>	Tyrosol-sulfate	Urine	3	ESI-	[M-H]	3.49	217.0172	217.0176	0.4
				ESI-	[M-H-sulfate]	3.50	137.0606	-	-

<b>98</b>	3-(3-hydroxyphenyl)propanoic acid	Urine	1	ESI-	[M-H]	3.50	165.0550	165.0530	2.0
<b>99</b>	N-lactoyl-Leucine	Urine	3	ESI-	[M-H]	3.50	202.1081	202.1085	0.4
<b>100</b>	Heptanoylcarnitine	Urine	3	ESI+	[M+H]	3.51	274.2024	274.2013	1.1
<b>101</b>	Phenyllactic acid	Faeces	1	ESI-	[M-H]	3.52	165.0548	165.0552	0.4
				ESI-	[M-H-CO <sub>2</sub> ]	3.51	121.0653	-	-
				ESI-	[M-H-HCOOH]	3.52	119.0494	119.0497	0.3
<b>102</b>	5-Butyltetrahydro-2-oxo-3-furancarboxylic acid	Urine	3	ESI-	[M-H]	3.53	185.0813	185.0819	0.6
				ESI-	[M-H] fragment (C <sub>8</sub> H <sub>12</sub> O)	3.53	123.0810	123.0815	0.5
<b>103</b>	Octenoylcarnitine	Urine	3	ESI+	[M+H]	3.55	286.2026	286.2013	1.3
				ESI+	[M+H] fragment	3.55	227.1287	-	-
				ESI+	[M+H] fragment	3.56	85.0289	-	-
<b>104</b>	Indolelactic acid	Urine	1	ESI-	[M-H]	3.56	204.0662	204.0649	1.3
				ESI+	[M+H-H <sub>2</sub> O-C <sub>2</sub> H <sub>2</sub> O <sub>2</sub> ]	3.57	130.0659	130.0663	0.4
<b>105</b>	Indoleacrylic glycine	Faeces; Urine	1	ESI-	[M-H]	3.56	243.0771	243.0764	0.7
				ESI-	[M-H-CO <sub>2</sub> ]	3.59	199.0964	199.0892	7.2
				ESI-	[M-H] fragment	3.57	168.0445	168.0448	0.3
				ESI-	[M-H] fragment	3.56	142.0658	142.0652	0.6
				ESI-	[M-H] fragment	3.56	100.0034	100.0020	1.4
				ESI+	[M+H] fragment	3.56	170.0549	170.0565	1.6
<b>106</b>	Indole-3-methyl acetate	Urine	3	ESI+	[M+H]	3.57	190.0874	190.0863	1.1
<b>107</b>	Gentisein	Faeces	3	ESI-	[M-H]	3.59	243.0301	243.0299	0.2

<b>108</b>	Indoleacetic acid	Serum	1	ESI+	[M-H-CO <sub>2</sub> ]	3.63	130.0654	130.0650	0.4	
<b>109</b>	Azelaic acid	Faeces	1	ESI-	[M-H]	3.66	187.0971	187.0971	0.0	
<b>110</b>	Urolithin C	Faeces	1	ESI-	[M-H]	3.67	243.0287	243.0289	0.2	
<b>111</b>	Nonanoylcarnitine	Urine	3	ESI+	[M+H]	3.73	302.2337	302.2326	1.1	
				ESI+	[M+H] fragment	3.73	243.1601	-	-	
				ESI+	[M+H] fragment	3.74	141.1281	-	-	
				ESI+	[M+H] fragment	3.73	85.0288	-	-	
				ESI+	[M+H] fragment	3.74	60.0807	-	-	
<b>112</b>	Urolithin A	Faeces	1	ESI-	[M-H]	3.74	227.0351	227.0340	-	1.1
<b>113</b>	Deoxypyridinoline	Urine	3	ESI-	[M+Cl]	3.74	447.1690	447.1652	3.8	
<b>114</b>	Urobilin / Urobilinogen	Faeces	3	ESI-	[M-H]	3.75	589.3033	589.3032	0.1	
<b>115</b>	Stercobilin	Faeces	3	ESI-	[M-H]	3.77	593.3343	593.3345	0.2	
<b>116</b>	Indolepropionic acid	Serum	1	ESI+	[M+H-C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> ]	3.77	130.0656	130.0644	1.2	
<b>117</b>	3-Carboxy-4-methyl-5-propyl-2-furanpropionic acid-glucuronide	Urine	3	ESI-	[M-H]	3.77	415.1252	415.1246	0.6	
<b>118</b>	3-hydroxyundecanoyl carnitine	Urine	3	ESI+	[M+H-H <sub>2</sub> O]	3.92	328.2489	328.2488	0.1	
				ESI+	[M+H] fragment	3.93	269.1754	-	-	
<b>119</b>	Dehydroisoandrosterone 3-sulfate	Serum	1	ESI-	[M-H]	4.04	367.1572	367.1570	0.2	
<b>120</b>	Glucarubin	Urine	3	ESI-	[M-H]	4.05	495.2225	495.2235	1.0	
<b>121</b>	3-Carboxy-4-methyl-5-propyl-2-furanpropionic acid	Serum; Urine	1	ESI-	[M-H]	4.05	239.0911	239.0901	1.0	

				ESI+	[M+H] fragment	4.05	181.0857	181.0869		1.2
<b>122</b>	Dodecanedioic acid	Urine	3	ESI-	[M-H]	4.08	229.1446		229.1445	0.1
<b>123</b>	Glycocholic acid	Faeces; Serum; Urine	1	ESI-	[M-H]	4.27	464.2991	464.3012		2.1
				ESI+	[M+H-H <sub>2</sub> O]	4.31	448.3066	448.3060		0.6
				ESI+	[M+H-2H <sub>2</sub> O]	4.25	430.2948	430.2959		1.1
				ESI+	[M+H] fragment	4.22	373.2695	373.2710		1.5
<b>124</b>	Muricholic acid	Faeces	3	ESI-	[M-H]	4.23	407.2802		407.2803	0.1
<b>125</b>	7-Ketodeoxycholic acid / 3-Oxocholeic acid	Faeces	3	ESI-	[M-H]	4.25	405.2640		405.2646	0.6
<b>126</b>	Glycochenodeoxycholic acid 3-sulfate	Urine	1	ESI-	[M-H]	4.44	528.2621	528.2635		1.4
<b>127</b>	Ursodeoxycholic acid	Faeces	1	ESI-	[M-H]	4.45	391.2851	391.2849	391.2854	0.2
<b>128</b>	Glycochenodeoxycholic acid	Serum	1	ESI+	[M+H-2H <sub>2</sub> O]	4.46	414.3013	414.3004		0.9
<b>129</b>	Cholic acid	Faeces; Serum; Urine	1	ESI-	[M-H]	4.46	407.2793	407.2798		0.5
<b>130</b>	Hyodeoxycholic acid	Faeces	1	ESI-	[M-H]	4.56	391.2838	391.2849		1.1
<b>131</b>	Chenodeoxycholic acid	Faeces	1	ESI-	[M-H]	4.63	391.2849	391.2849		0.0
<b>132</b>	12-Ketodeoxycholic acid or similar	Faeces	4	ESI-	[M-H]	4.71	389.2697		389.2697	0.0
<b>133</b>	Deoxycholic acid	Faeces	1	ESI-	[M-H]	4.73	391.2846	391.2849		0.3

\* We noted a modest retention time shift (<0.1 min) when comparing the retention times of the initial analyses with the retention times obtained when analysing authentic standards. However, for a few compounds (Phenol sulfate and Indoxyl-sulfate) this shift was more pronounced (rt shift = 0.2-0.3 min).

†Identification levels by Metabolomics Standard Initiative.[1] ESI, electrospray ionization; rt, retention time; *m/z*, mass-to-charge.

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**References**

1. Sumner LW, Amberg A, Barrett D, *et al.* Proposed minimum reporting standards for chemical analysis. *Metabolomics* 2007;**3**:211–21.