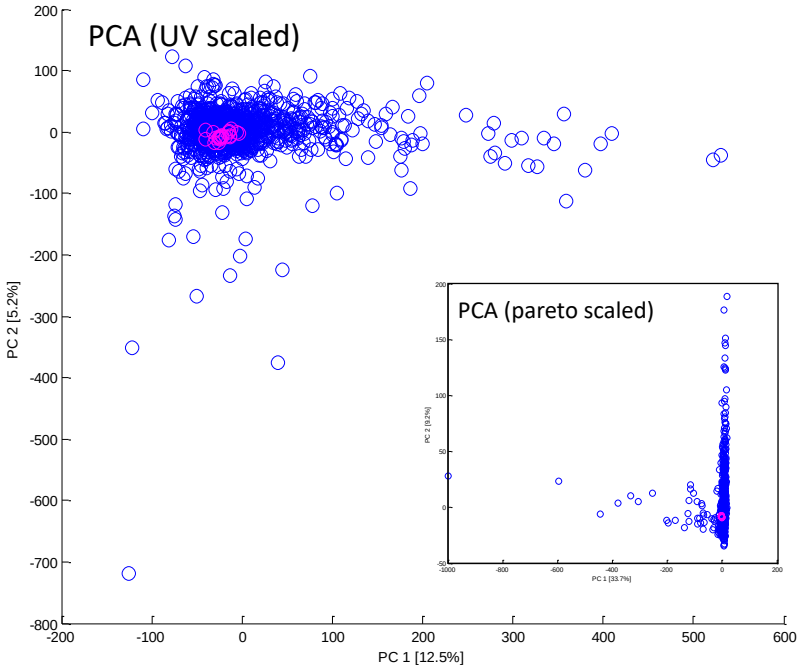
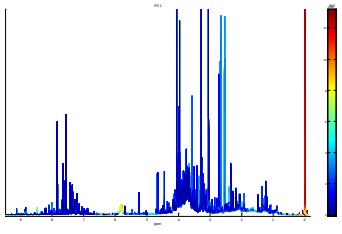
**Supplemental Information 1: Quality assessment of the dataset**

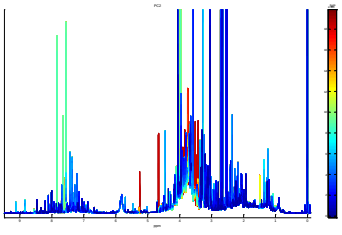
PCA analysis was carried out to investigate the main variations in the dataset (Figure 1). We used the dataset with chemical shifts ranging from -0.5 to 9.5 ppm and excluded the water peak between 4.7-5.00 ppm. The two first components (PC1 12.5 and PC2 5.2%) showed the internal standard TSP (see Figure 2, e.g. urine dilution) and urinary glucose (Figure 2, i.e. glucosuria) as main contributors of variation. Similarly, pareto-scaled PCA analysis revealed the same drivers in the principal component, the percentage of variation was higher (PC1 33.2%, PC2 9.2%). We did not observe evidence for technical outliers such as spectral quality (i.e. baseline variation, water suppression issues) and processing quality (i.e. alignment, normalization)).




PC 1 : „urine dilution“ (TSP)



PC 2 : glucosuria (e.g. diabetes)



SI Figure S1: PCA analysis showing main contribution in the PCA plots (both univariate and pareto scaling) from amounts of internal standard TSP (relative to metabolites, showing the urine dilution) and glucose (highlighting glucosuria mainly from diabetes patients).

**Supplemental Information 2: Salicyluric acid**

In order to confirm the identity of salicyluric acid (SUA) we conducted a spiking experiment of the chemical standards and salicylic acid (SA) into pure urine. Figure 1 shows the pure standards and spikings in different concentrations. We conducted the spiking as a series spiking, i.e. analysis of pure urine, then spiking of the first standard (5µL SUA) with immediate analysis, followed by spiking of 5 µL SA and analysis. Lastly, we respiked 10 µL of SUA to reconfirm a further rise of the resonances seen after 5 µL of SUA. Indeed, chemical shifts of SUA and SA are similar but distinguishable and match the chemical shifts seen in our dataset.

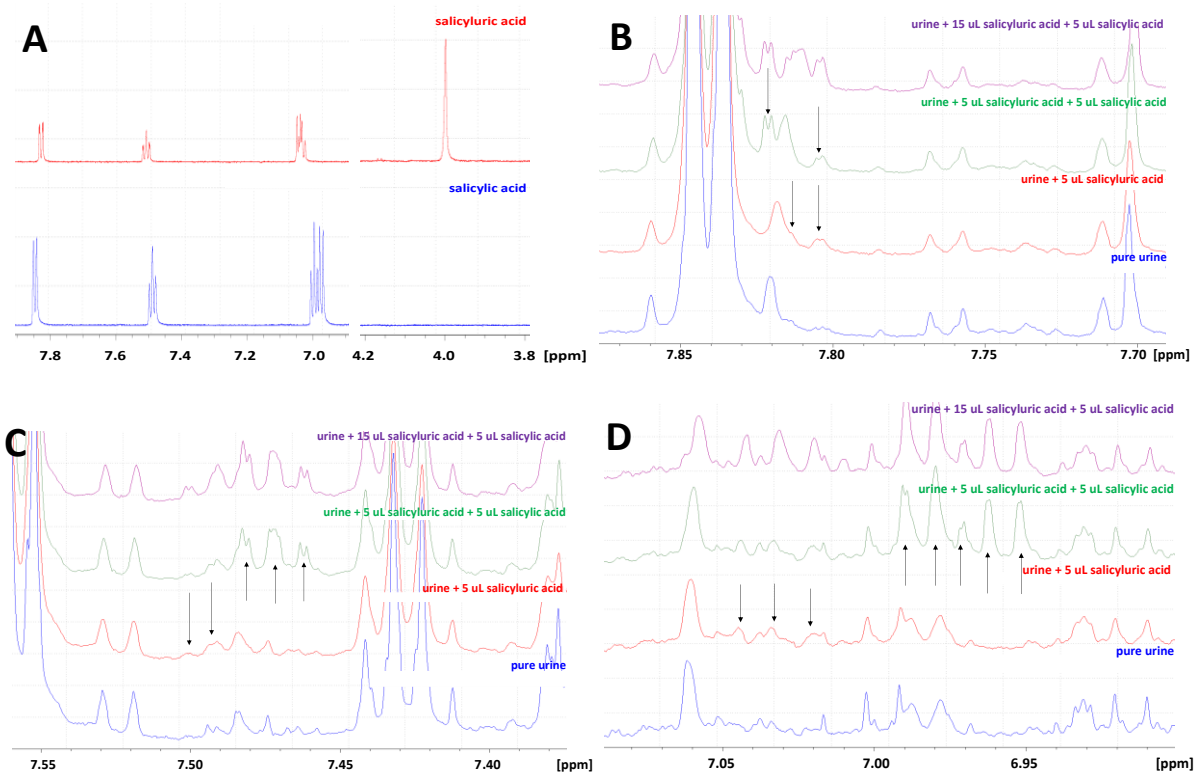



**Figure S2:** Spiking experiment of salicyluric acid and salicylic acid to human urine (QC sample). (**A**) pure standard samples of salicyluric acid and salicylic acid, (**B-D**) 1H NMR spectra of pure urine and urine with addition of 5 uL salicyluric acid (0.5 mg/mL), 5 uL salicylic acid (1.2 mg/mL) and 15 uL salicyluric acid (0.5 mg/mL) + 5uL salicylic acid (1.2 mg/mL) with highlight of the appearing resonances by arrows.

OPLS-DA analysis of per n-fold plot identified SUA excreters vs all other individuals highlighted all resonances from SUA and additional resonances from glucuronidated salicylic acid metabolites and paracetamol.

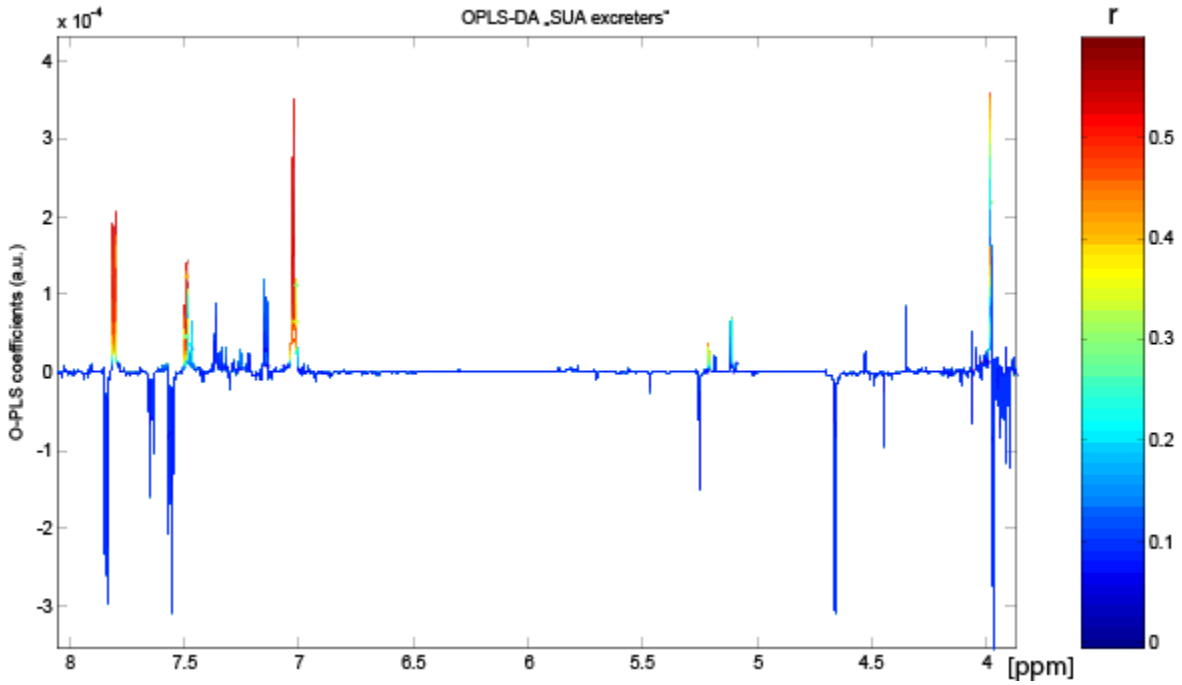



**Figure S3:** Loadings plot of OPLS-DA analysis comparing SUA excreters with all other individuals. THE SUA resonances (δ 7.806 dd, 7.49 ddd, 7.022 m, 3.98s ppm). Additional resonances appear at δ 5.11 (d) and 5.21 (d).

**Supplemental Information 3: Experimental details for Sample preparation and acquisition of NMR spectra**

*Automated sample preparation protocol for urine samples*

- Overnight thawing in the fridge at 4 °C
- Vortex sample
- Transfer of 150 µL to Eppendorf using Hamilton Microlab STAR® liquid handler
- Simultaneous production of QC:
    - 5 µL of every sample to pool
    - Vortex and split into "samples" of 150 µL each (n = 1000 samples -> 5 mL -> 33 QCs)
- Addition of phosphate buffer (50 µL) and KF (10 µL):
    - $PO_4$ buffer: 100% $D_2O$, 0.1% TSP, 2 mM $NaN_3$, pH 7.4
    - KF buffer: 4.5 M KF in 100% $D_2O$
- Gentle mixing by 3x inversion
- Store in fridge till analysis (max 24 hours) or in freezer at -80 °C
- Vortex and centrifugation (12,000 rpm for 10 min at 4°C)
- Transfer to 3 mm NMR tubes
- Air-tight sealing
- Analysis by NMR spectroscopy

*NMR spectroscopy*

Pulse program: noesygppr1d

Size of fid: 64K

Dummy scans: 16

Scans: 256

Sweep width: 16 ppm

Acquisition time: 3s

Mixing time: 200 ms

90° pulse (p1): 13 µsec

Relaxation (d1): 4 s

Receiver gain: 45.2

Dwell time: 39 µsec

Line broadening: 0.3

Temperature: 300K

SI_Table_S1

| # | ppm shift | metabolite annotation | HMDB ID |
|---|---|---|---|
| 1 | 7.4400 | phenylacetylglutamine | HMDB0006344 |
| 2 | 7.3548 | phenylacetylglutamine | HMDB0006344 |
| 3 | 7.3790 | phenylacetylglutamine | HMDB0006344 |
| 4 | 2.2760 | phenylacetylglutamine | HMDB0006344 |
| 5 | 2.2658 | phenylacetylglutamine | HMDB0006344 |
| 6 | 7.4308 | phenylacetylglutamine | HMDB0006344 |
| 7 | 7.3633 | phenylacetylglutamine | HMDB0006344 |
| 8 | 2.1208 | phenylacetylglutamine | HMDB0006344 |
| 9 | 2.1033 | phenylacetylglutamine | HMDB0006344 |
| 10 | 1.9328 | phenylacetylglutamine | HMDB0006344 |
| 11 | 1.9243 | phenylacetylglutamine | HMDB0006344 |
| 12 | 4.1695 | phenylacetylglutamine | HMDB0006344 |
| 13 | 4.1745 | phenylacetylglutamine | HMDB0006344 |
| 14 | 2.2848 | phenylacetylglutamine | HMDB0006344 |
| 15 | 2.1135 | phenylacetylglutamine | HMDB0006344 |
| 16 | 2.1090 | phenylacetylglutamine | HMDB0006344 |
| 17 | 2.0933 | phenylacetylglutamine | HMDB0006344 |
| 18 | 1.9518 | phenylacetylglutamine | HMDB0006344 |
| 19 | 1.9413 | phenylacetylglutamine | HMDB0006344 |
| 20 | 1.9150 | phenylacetylglutamine | HMDB0006344 |
| 21 | 1.9048 | phenylacetylglutamine | HMDB0006344 |
| 22 | 2.1265 | phenylacetylglutamine | HMDB0006344 |
| 23 | 7.4213 | phenylacetylglutamine | HMDB0006344 |
| 24 | 3.6815 | phenylacetylglutamine | HMDB0006344 |
| 25 | 3.6580 | phenylacetylglutamine | HMDB0006344 |
| 26 | 4.1833 | phenylacetylglutamine | HMDB0006344 |
| 27 | 4.1900 | phenylacetylglutamine | HMDB0006344 |
| 28 | 8.0023 | phenylacetylglutamine | HMDB0006344 |
| 29 | 2.1365 | phenylacetylglutamine | HMDB0006344 |
| 30 | 2.0993 | phenylacetylglutamine | HMDB0006344 |
| 31 | 2.1308 | phenylacetylglutamine | HMDB0006344 |
| 32 | 6.7863 | phenylacetylglutamine | HMDB0006344 |
| 33 | 5.0910 | p-cresol-glucuronide | HMDB0011686 |
| 34 | 5.0815 | p-cresol-glucuronide | HMDB0011686 |
| 35 | 7.2915 | p-cresol-sulfate | HMDB0011635 |
| 36 | 7.2815 | p-cresol-sulfate | HMDB0011635 |
| 37 | 7.2223 | p-cresol-sulfate | HMDB0011635 |
| 38 | 7.2188 | p-cresol-sulfate | HMDB0011635 |

| | | | |
|---|---|---|---|
| 39 | 7.2083 | p-cresol-sulfate | HMDB0011635 |
| 40 | 2.3478 | p-cresol-sulfate | HMDB0011635 |
| 41 | 2.3008 | p-cresol-glucuronide | HMDB0011686 |
| 42 | 3.6395 | phenylacetylglutamine | HMDB0006344 |
| 43 | 7.9925 | phenylacetylglutamine | HMDB0006344 |
| 44 | 4.1635 | phenylacetylglutamine | HMDB0006344 |
| 45 | 7.7100 | indoxylsulfate | HMDB0000682 |
| 46 | 7.5230 | indoxylsulfate | HMDB0000682 |
| 47 | 7.5125 | indoxylsulfate | HMDB0000682 |
| 48 | 7.7003 | indoxylsulfate | HMDB0000682 |
| 49 | 7.3718 | indoxylsulfate | HMDB0000682 |
| 50 | 7.2760 | indoxylsulfate | HMDB0000682 |
| 51 | 7.4650 | quinolinic acid | HMDB0000232 |
| 52 | 7.4553 | quinolinic acid | HMDB0000232 |
| 53 | 7.4613 | quinolinic acid | HMDB0000232 |
| 54 | 7.2330 | | |
| 55 | 7.2285 | | |
| 56 | 2.3420 | p-cresol-sulfate | HMDB0011635 |
| 57 | 7.2575 | 3-hydroxyphenylacetate | HMDB0000440 |
| 58 | 7.2480 | 3-hydroxyphenylacetate | HMDB0000440 |
| 59 | 7.2543 | 3-hydroxyphenylacetate | HMDB0000440 |
| 60 | 6.8098 | 3-hydroxyphenylacetate | HMDB0000440 |
| 61 | 6.8020 | 3-hydroxyphenylacetate | HMDB0000440 |
| 62 | 7.2685 | 3-hydroxyphenylacetate | HMDB0000440 |
| 63 | 6.7430 | cinnamoylglycine | HMDB0011621 |
| 64 | 6.7230 | cinnamoylglycine | HMDB0011621 |
| 65 | 7.9080 | | |
| 66 | 7.0420 | | |
| 67 | 6.8810 | 4-hydroxyphenylacetate | HMDB0060390 |
| 68 | 6.8703 | 4-hydroxyphenylacetate | HMDB0060390 |
| 69 | 7.1748 | 4-hydroxyphenylacetate | HMDB0060390 |
| 70 | 7.1640 | 4-hydroxyphenylacetate | HMDB0060390 |
| 71 | 3.4525 | 4-hydroxyphenylacetate | HMDB0060390 |
| 72 | 3.3515 | | |
| 73 | 3.2768 | trimethylamine-N-oxide | HMDB0000925 |
| 74 | 7.4915 | | |
| 75 | 7.4808 | | |
| 76 | 7.4715 | | |
| 77 | 7.3333 | | |
| 78 | 7.3428 | | |
| 79 | 7.8120 | salicyluric acid | HMDB0000840 |

| | | | |
|---|---|---|---|
| 80 | 7.8000 | salicyluric acid | HMDB0000840 |
| 81 | 7.4995 | salicyluric acid | HMDB0000840 |
| 82 | 7.0313 | salicyluric acid | HMDB0000840 |
| 83 | 7.0223 | salicyluric acid | HMDB0000840 |
| 84 | 7.0158 | tea metabolite | |
| 85 | 7.0125 | tea metabolite | |
| 86 | 8.7970 | N-methylpyridinium | HMDB0240545 |
| 87 | 8.7905 | N-methylpyridinium | HMDB0240545 |
| 88 | 4.4060 | N-methylpyridinium | HMDB0240545 |
| 89 | 1.8930 | quinic acid | HMDB0003072 |
| 90 | 1.8795 | quinic acid | HMDB0003072 |
| 91 | 1.8628 | quinic acid | HMDB0003072 |
| 92 | 9.1280 | trigonelline | HMDB00875 |
| 93 | 8.8505 | trigonelline | HMDB00875 |
| 94 | 8.8413 | trigonelline | HMDB00875 |
| 95 | 8.0950 | trigonelline | HMDB00875 |
| 96 | 4.4465 | trigonelline | HMDB00875 |
| 97 | 8.0858 | trigonelline | HMDB00875 |
| 98 | 8.1038 | trigonelline | HMDB00875 |
| 99 | 1.9798 | quinic acid | HMDB0003072 |
| 100 | 1.9750 | quinic acid | HMDB0003072 |
| 101 | 1.9835 | quinic acid | HMDB0003072 |
| 102 | 1.9650 | quinic acid | HMDB0003072 |
| 103 | 1.9600 | quinic acid | HMDB0003072 |
| 104 | 1.9565 | quinic acid | HMDB0003072 |
| 105 | 1.9713 | quinic acid | HMDB0003072 |
| 106 | 9.0563 | 5-acetylamino-6-formylamino-3-methyluracil | HMDB0011105 |
| 107 | 2.1910 | 5-acetylamino-6-formylamino-3-methyluracil | HMDB0011105 |
| 108 | 3.2050 | 5-acetylamino-6-amino-3-methyluracil | HMDB0004400 |
| 109 | 2.1773 | 5-acetylamino-6-amino-3-methyluracil | HMDB0004400 |
| 110 | 1.8708 | quinic acid | HMDB0003072 |
| 111 | 7.9363 | | |
| 112 | 3.3238 | | |
| 113 | 1.0825 | unknown, coffee cluster | |
| 114 | 1.0740 | unknown, coffee cluster | |
| 115 | 1.0323 | unknown, coffee cluster | |
| 116 | 0.9803 | | |
| 117 | 8.2293 | | |
| 118 | 3.3878 | | |
| 119 | 7.8543 | unknown, coffee cluster | |
| 120 | 3.0028 | | |

| | | | |
|---|---|---|---|
| 121 | 8.0268 | | |
| 122 | 7.1305 | 3-hydroxyhippurate | HMDB06116 |
| 123 | 7.1275 | 3-hydroxyhippurate | HMDB06116 |
| 124 | 6.9898 | 4-hydroxyhippurate | HMDB13678 |
| 125 | 6.9800 | 4-hydroxyhippurate | HMDB13678 |
| 126 | 6.8643 | (3-hydroxyphenyl)-3-hydroxypropionic acid | HMDB02643 |
| 127 | 6.8540 | (3-hydroxyphenyl)-3-hydroxypropionic acid | HMDB02643 |
| 128 | 6.9300 | (3-hydroxyphenyl)-3-hydroxypropionic acid | HMDB02643 |
| 129 | 5.0103 | (3-hydroxyphenyl)-3-hydroxypropionic acid | HMDB02643 |
| 130 | 7.1215 | 3-hydroxyhippurate | HMDB06116 |
| 131 | 7.1185 | 3-hydroxyhippurate | HMDB06116 |
| 132 | 7.4110 | 3-hydroxyhippurate | HMDB06116 |
| 133 | 7.3035 | (3-hydroxyphenyl)-3-hydroxypropionic acid | HMDB06116 |
| 134 | 3.9488 | 3-/4-hydroxyhippurate | HMDB06116/HMDB02643 |
| 135 | 2.6998 | (3-hydroxyphenyl)-3-hydroxypropionic acid | HMDB02643 |
| 136 | 7.3135 | 3-hydroxyhippurate | HMDB06116 |
| 137 | 6.9270 | (3-hydroxyphenyl)-3-hydroxypropionic acid | HMDB02643 |
| 138 | 2.6273 | (3-hydroxyphenyl)-3-hydroxypropionic acid | HMDB02643 |
| 139 | 2.6198 | (3-hydroxyphenyl)-3-hydroxypropionic acid | HMDB02643 |
| 140 | 2.6015 | (3-hydroxyphenyl)-3-hydroxypropionic acid | HMDB02643 |
| 141 | 5.0278 | (3-hydroxyphenyl)-3-hydroxypropionic acid | HMDB02643 |
| 142 | 5.0205 | (3-hydroxyphenyl)-3-hydroxypropionic acid | HMDB02643 |
| 143 | 7.5918 | unknown, hydroxyhippurate-cluster | |
| 144 | 7.5815 | unknown, hydroxyhippurate-cluster | |
| 145 | 7.3235 | 3-hydroxyhippurate | HMDB06116 |
| 146 | 7.3100 | 3-hydroxyhippurate | HMDB06116 |
| 147 | 7.7465 | 4-hydroxyhippurate | HMDB13678 |
| 148 | 7.7350 | 4-hydroxyhippurate | HMDB13678 |
| 149 | 2.6895 | (3-hydroxyphenyl)-3-hydroxypropionic acid | HMDB02643 |
| 150 | 2.6088 | (3-hydroxyphenyl)-3-hydroxypropionic acid | HMDB02643 |
| 151 | 6.9943 | 4-hydroxyhippurate | HMDB13678 |
| 152 | 6.9835 | 4-hydroxyhippurate | HMDB13678 |
| 153 | 7.7570 | 4-hydroxyhippurate | HMDB13678 |
| 154 | 7.7680 | 4-hydroxyhippurate | HMDB13678 |
| 155 | 3.9443 | 3-/4-hydroxyhippurate | HMDB06116/HMDB02643 |
| 156 | 3.9530 | 3-/4-hydroxyhippurate | HMDB06116/HMDB02643 |
| 157 | 7.6043 | unknown, hydroxyhippurate-cluster | |
| 158 | 7.6328 | hippurate | HMDB00714 |
| 159 | 7.5455 | hippurate | HMDB00714 |
| 160 | 7.8448 | hippurate | HMDB00714 |
| 161 | 7.8358 | hippurate | HMDB00714 |

| | | | |
|---|---|---|---|
| 162 | 7.6558 | hippurate | HMDB00714 |
| 163 | 7.6463 | hippurate | HMDB00714 |
| 164 | 7.6370 | hippurate | HMDB00714 |
| 165 | 7.5698 | hippurate | HMDB00714 |
| 166 | 7.5595 | hippurate | HMDB00714 |
| 167 | 7.5500 | hippurate | HMDB00714 |
| 168 | 3.9753 | hippurate | HMDB00714 |
| 169 | 3.9683 | hippurate | HMDB00714 |
| 170 | 7.6605 | hippurate | HMDB00714 |
| 171 | 8.5560 | hippurate | HMDB00714 |
| 172 | 8.5455 | hippurate | HMDB00714 |
| 173 | 7.8688 | hippurate | HMDB00714 |
| 174 | 7.9403 | hippurate | HMDB00714 |
| 175 | 7.9305 | hippurate | HMDB00714 |
| 176 | 6.9675 | | |
| 177 | 6.9625 | sumiki's acid | HMDB02432 |
| 178 | 6.9575 | | |
| 179 | 6.9470 | | |
| 180 | 6.9365 | | |
| 181 | 6.6065 | | |
| 182 | 6.8975 | | |
| 183 | 6.8875 | | |
| 184 | 7.4008 | tea metabolite | |
| 185 | 4.5078 | tea metabolite | |
| 186 | 6.9730 | tea metabolite | |
| 187 | 7.0658 | tea metabolite | |
| 188 | 7.3963 | tea metabolite | |
| 189 | 7.3880 | tea metabolite | |
| 190 | 7.0725 | tea metabolite | |
| 191 | 7.1133 | 3-hydroxyhippurate | HMDB06116 |
| 192 | 7.1043 | 3-hydroxyhippurate | HMDB06116 |
| 193 | 6.6953 | | |
| 194 | 6.6900 | | |
| 195 | 6.6698 | | |
| 196 | 6.3725 | | |
| 197 | 6.3925 | | |