Supplementary

**Online supplementary material** **Table S1.** ***Concentrations of selected odorants in native human urine.*** Displayed are the minimum, the maximum, and the median concentrations in the non-normalized form as well as normalized by creatinine concentration.

| **No.** 1 | **Compound** 2 | **Minimum concentration [µg/L]** | **Maximum concentration [µg/L]** | **Median concentration [µg/L]** | **Minimum concentration [µg/mol creatinine]** | **Maximum concentration [µg/mol creatinine]** | **Median concentration [µg/mol creatinine]** | **Number of samples** 3 |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 1 | oct-1-en-3-one | 0.03 | 0.13 | 0.08 | 1.32 | 34.5 | 10.4 | 5 // 7 |
| 2 | 4-ethylguaiacol | 0.04 | 1.47 | 0.26 | 4.39 | 386 | 43.9 | 7 // 8 |
| 3 | 4-vinylguaiacol | 0.62 | 2.80 | 1.06 | 42.9 | 501 | 290 | 5 // 4 |
| 4 | *(E)*-β-damascenone | 0.004 | 0.39 | 0.02 | 0.82 | 72.9 | 1.58 | 5 // 10 |
| 5 | dimethyl trisulfide | 0.08 | 1.02 | 0.20 | 8.99 | 177 | 52.4 | 6 // 0 |
| 6 | guaiacol | 0.04 | 0.54 | 0.13 | 4.29 | 96.2 | 33.6 | 5 // 5 |
| 7 | indole | 0.24 | 0.40 | 0.34 | 14.1 | 158 | 51.6 | 7 // 2 |
| 8 | methional | 0.26 | 1.34 | 0.51 | 32.5 | 239 | 82.3 | 8 // 2 |
| 9 | skatole | 0.06 | 0.30 | 0.10 | 4.79 | 60.3 | 27.8 | 9 // 0 |
| 10 | vanillin | 1.60 | 5.64 | 2.55 | 125 | 1,230 | 510 | 9 // 1 |

1.Numbering in accordance to online supplementary material Table S2; 2.Compounds listed in alphabetical order; 3.Determinations yielding values below or above the limit of quantification are separated from values within the calibration line by a double slash.

**Online supplementary material Table S2.** Selected ions, internal standards and chemical information on odorants in native human urine quantified by stable isotope dilution assays.

| **No.** 1 | **Compound** 2 | **Chemical formula** | **mass** | **Ion (m/z)** | **Internal standard** | **mass** | **Ion (m/z)** |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 1 | oct-1-en-3-one | C8H14O | 126 | 127 | [2H3]-oct-1-en-3-one | 129 | 130 |
| 2 | 4-ethylguaiacol | C9H12O2 | 152 | 153 | [2H5]- 4-ethylguaiacol | 157 | 158 |
| 3 | 4-vinylguaiacol | C9H10O2 | 150 | 151 | [2H3]- 4-vinylguaiacol | 153 | 154 |
| 4 | *(E)*-β-damascenone | C13H18O | 190 | 191 | [2H3-4]-*(E)*-β-damascenone | 193–194 | 195 |
| 5 | dimethyl trisulfide | C2H6S3 | 126 | 127 | [2H6]- dimethyl trisulfide | 132 | 133 |
| 6 | guaiacol | C7H8O2 | 124 | 125 | [2H3]-guaiacol | 127 | 128 |
| 7 | indole | C8H7N | 117 | 118 | [2H7]-indole | 124 | 124 |
| 8 | methional | C8H8OS | 104 | 105 | [2H3]-methional | 107 | 108 |
| 9 | skatole | C9H9N | 131 | 132 | [2H7]- skatole | 138 | 139 |
| 10 | vanillin | C8H8O3 | 152 | 153 | [13C6]- vanillin | 158 | 159 |

1 Numbering in accordance to online supplementary material Table S1; 2.Compounds listed in alphabetical order.

**Online supplementary material Table S3.** ***Concentrations of selected odorants in glucuronidase-treated human urine.*** Displayed are the minimum, the maximum, and the median concentrations in the non-normalized form as well as normalized by creatinine concentration.

| **No.** 1 | **Compound**2 | **Minimum concentration**  **[µg/L]** | **Maximum concentration**  **[µg/L]** | **Median concentration**  **[µg/L]** | **Minimum concentration**  **[µg/mol creatinine]** | **Maximum concentration**  **[µg/mol creatinine]** | **Median concentration**  **[µg/mol creatinine]** | **Number of samples**3 |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 1 | 3-methylbutanoic acid | 569 | 9,560 | 1,050 | 38,700 | 1,800,000 | 174,000 | 12 // 0 |
| 2 | 4-ethylguaiacol | 3.53 | 77.0 | 6.88 | 322 | 8,760 | 952 | 5 // 6 |
| 3 | 4-vinylguaiacol | 16.3 | 171 | 46.9 | 1,000 | 89,000 | 7,890 | 8 // 6 |
| 4 | *(E)*-β-damascenone | 0.26 | 0.47 | 0.39 | 25.2 | 72.9 | 51.9 | 3 // 12 |
| 5 | butanoic acid | 272 | 784 | 346 | 32,000 | 168,000 | 61,100 | 11 // 1 |
| 6 | dimethyl trisulfide | 3.93 | 8.80 | 6.74 | 402 | 1,660 | 855 | 7 // 1 |
| 7 | guaiacol | 45.8 | 438 | 122 | 5,690 | 52,400 | 22,000 | 9 // 1 |
| 8 | indole | 34.1 | 287 | 186 | 13,400 | 49,100 | 33,200 | 7 // 2 |
| 9 | methional | 1.16 | 7.94 | 3.72 | 54.3 | 1,530 | 904 | 7 // 3 |
| 10 | skatole | 0.32 | 1.11 | 0.54 | 15.2 | 198 | 96.9 | 6 // 3 |
| 11 | sotolone | 31.5 | 434 | 88.1 | 5,990 | 226,000 | 10,800 | 4 // 11 |
| 12 | vanillin | 18.5 | 45.3 | 33.1 | 2,120 | 8,860 | 6,300 | 6 // 4 |

.Numbering in accordance to online supplementary material Table S4; 2.Compounds listed in alphabetical order; 3.Determinations yielding values below or above the limit of quantification are separated from values within the calibration line by a double slash.

**Online supplementary material Table S4.** Selected ions, internal standards and chemical information on odorants in glucuronidase-treated human urine quantified by stable isotope dilution assays.

| **No. 1** | **Compound 2** | **Chemical formula** | **mass** | **Ion (m/z)** | **Internal standard** | **mass** | **Ion (m/z)** |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 1 | 3-methylbutanoic acid | C5H10O2 | 102 | 60 | 2,2-[2H2]-3-methylbutanoic acid | 104 | 62 |
| 2 | 4-ethylguaiacol | C9H12O2 | 152 | 153 | [2H5]- 4-ethylguaiacol | 157 | 158 |
| 3 | 4-vinylguaiacol | C9H10O2 | 150 | 151 | [2H3]- 4-vinylguaiacol | 153 | 154 |
| 4 | *(E)*-β-damascenone | C13H18O | 190 | 191 | [2H3-4]-*(E)*-β-damascenone | 193–194 | 195 |
| 5 | butanoic acid | C4H8O2 | 88 | 60 | [13C2]- butanoic acid | 90 | 62 |
| 6 | dimethyl trisulfide | C2H6S3 | 126 | 127 | [2H6]- dimethyl trisulfide | 132 | 133 |
| 7 | guaiacol | C7H8O2 | 124 | 125 | [2H3]-guaiacol | 127 | 128 |
| 8 | indole | C8H7N | 117 | 118 | [2H7]-indole | 124 | 124 |
| 9 | methional | C8H8OS | 104 | 105 | [2H3]-methional | 107 | 108 |
| 10 | skatole | C9H9N | 131 | 132 | [2H7]- skatole | 138 | 139 |
| 11 | sotolone | C6H8O3 | 128 | 129 | [13C2]- sotolone | 130 | 131 |
| 12 | vanillin | C8H8O3 | 152 | 153 | [13C6]- vanillin | 158 | 159 |

1.Numbering in accordance to online supplementary material Table S3; 2.Compounds listed in alphabetical order.