**Supplementary table 12 | List of significantly associated metabolites whose excretion discriminates between athletes and controls when using LC-MS metabolic profiling models of urine (Supplementary figure 2A-D).**

Lists the metabolite name, liquid chromatography (LC)-platform, mass charge ratio (m/z), MSMS fragments, retention time (RT), level of assignment (LoA) and direction of association (↑ indicates higher excretion in the athletes group, ↓ indicates lower excretion in the athletes group) in urine.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Metabolite** | **LC-platform** | **m/z** | **MSMS product ions (5-20eV)** | **RT** | **LoA** | **Association** |
| N-formylanthranilic acid | RP - | 164.034 | 120.04, 136.04, 92.05 | 4.52 | 2 | ↑ |
| Hydantoin-5-propionic acid | RP - | 171.040 | 100.04, 127.06, 128.04 | 1.43 | 2 | ↑ |
| 3-Carboxy-4-methyl-5-propyl-2-furanpropionic acid (CMPF) | RP - | 239.091 | 195.10, 151.11 | 6.16 | 2 | ↑ |
| CMPF glucuronide x1 | RP - | - | Aglycone: CMPF *(239.09 – see above)* | - | \* | ↑ |
| Trimetaphosphoric acid | RP - | 238.891 | 96.96, 220.90, 78.96 | 0.42 | 2 | ↑ |
| Glucuronide x1 | RP - | - | Aglycone: 239.09 | - | \* | ↑ |
| Acetylcarnitine - C2 | RP + | 204.125 | 145.05, 85.03 | 0.85 | 2 | ↑ |
| Propionylcarnitine - C3 | RP + | 218.139 | 159.07, 85.03 | 1.99 | 2 | ↑ |
| (Iso)Butyrylcarnitine - C4 | RP + | 232.155 | 173.08. 85.03 | 2.83 | 2 | ↑ |
| 2-Methylbutyroylcarnitine - C5 | RP + | 246.171 | 187.10, 85.03 | 3.60 | 2 | ↑ |
| C9:1-carnitine | RP + | 300.217 | 241.14, 139.11, 85.03 | 5.32 | 2 | ↑ |
| L-Valine | RP + | 118.086 | 72.08 | 2.43 | 2 | ↑ |
| Nicotinuric acid | RP + | 181.061 | 135.06 | 3.33 | 2 | ↑ |
| Hexanoylcarnitine - C6 | HILIC + | 260.185 | 201.11, 85.03 | 5.72 | 2 | ↑ |
| 4-Pyridoxic acid | HILIC + | 184.062 | 166.05, 148.04, 138.06 | 1.14 | 2 | ↑ |
| Creatinine | HILIC + | 114.067 | 87.06 | 6.49 | 2 | ↑ |
| Glutamine | RP - | 145.061 | 127.05, 102.95, 101.94, 128.04, 84.05, 109.04 | 2.89 | 2 | ↓ |
| Unknown glucuronides x9 | RP - | - | Aglycones: 195.06, 271.07, 285.12, 237.14, 209.12, 143.07, 269.18, 257.17, 217.06 | - | \* | ↓ |
| 7-Methylxanthine | RP + | 167.059 | 124.05, 150.03, 142.06 | 1.98 | 2 | ↓ |
| Imidazoleacetic acid | RP + | 127.051 | 81.05 | 0.67 | 2 | ↓ |
| Isoquinoline / quinoline | RP + | 130.065 | 103.06 | 4.79 | 2 | ↓ |
| Unknown glucuronides x7 | RP + | - | Aglycones: 303.15, 219.06, 297.14, 383.14, 281.17, 239.16, 265.18 | - | \* | ↓ |

The Level of Assignment (LoA) used for the molecules identified by MS are LoA 1: Identified compound, confirmed by comparison to an authentic chemical reference. LoA 2: MS/MS spectrum matched to database or literature to putatively annotate compound.

\*Glucuronides characterised by a neutral loss of 176.03 Da (loss of monodehydrated glucuronic acid) in positive and negative modes. Further characterised by 175 m/z (anhydrous glucuronic acid) + 113 m/z (fragment of glucuronic acid) product ions in negative mode. If unable to unambiguously identify resulting aglycone, aglycone m/z stated.