

Figure S1: Chromatogram of the organic acid analysis of the case study sample. Due to the complexity of the chromatogram above, it has been divided into six segments (A–F) and given in more detail in the corresponding figures below. The y-axis is the percentage abundance (relative to the most abundant peak in the total ion chromatogram), and the x-axis is the retention time in minutes.

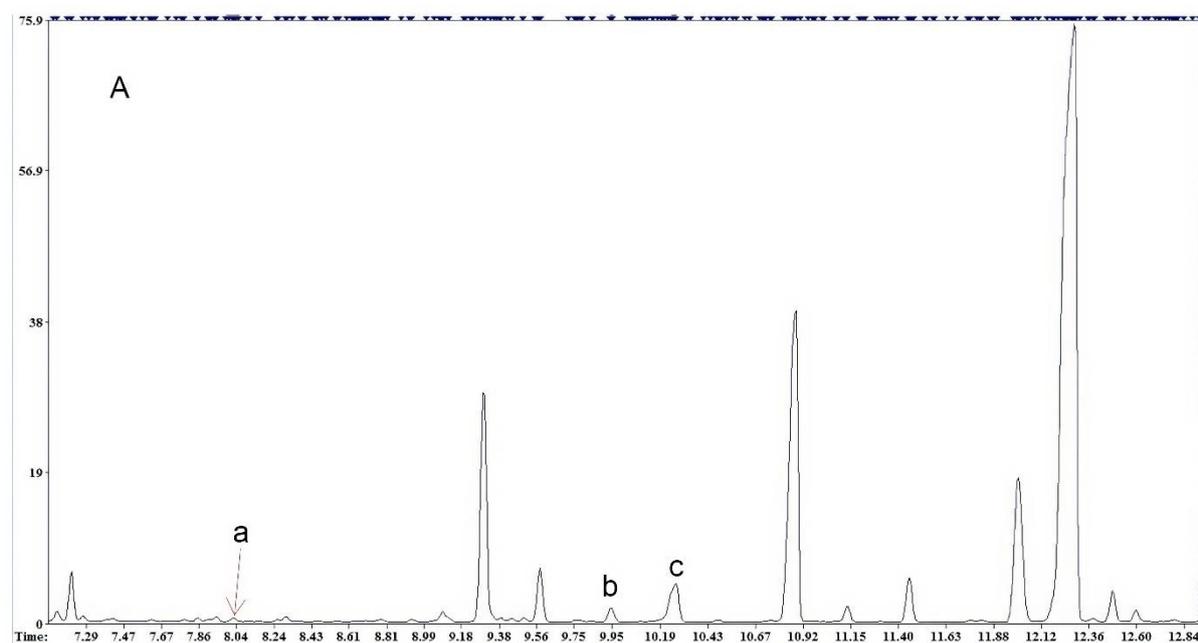


Figure S2: Segment A of Figure S1. The compound list is as follows: (a) 2-ketoisovaleric acid (mono-TMS ester), (b) pyruvate and (c) 2-keto-3-methylvaleric acid. The y-axis (abundance) is scaled to the most abundant peak of this segment and the x-axis (retention time in minutes) is cropped to only show segment A as indicated in Figure S1.

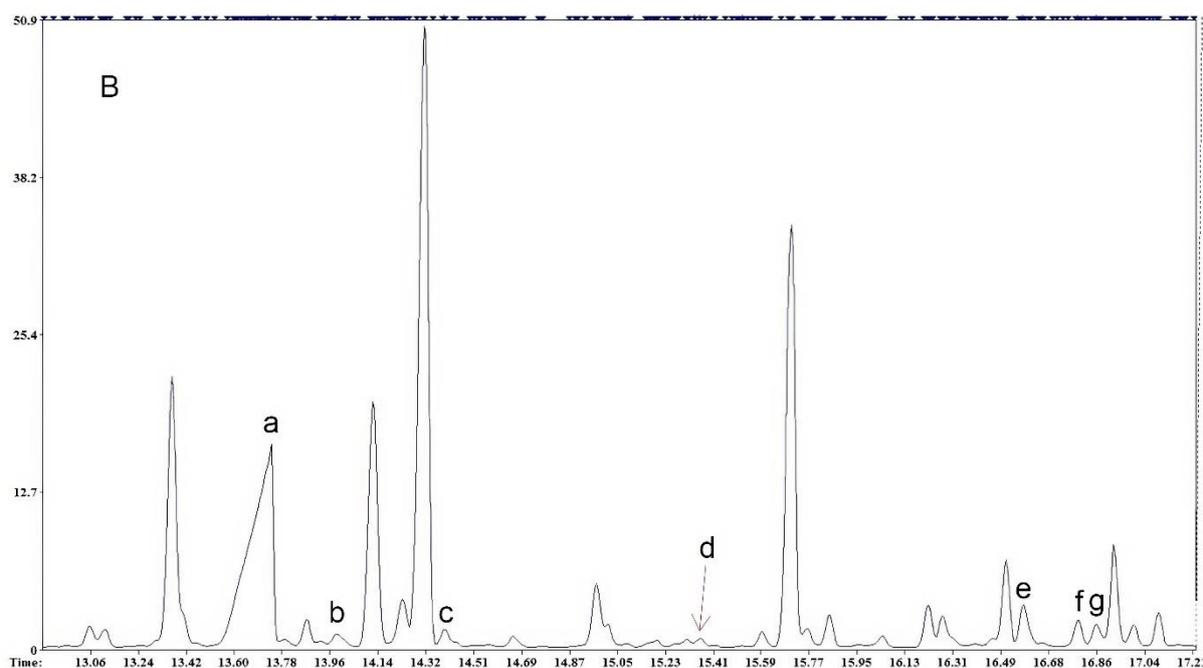


Figure S3: Segment B of Figure S1. The compound list is as follows: (a) urea, (b) N-Ac-Ala, (c) 2-ketoisocaproic acid, (d) 2-ketoisovaleric acid (di-TMS ester), (e) 2-ketovaleric acid, (f) N-Ac-Val (mono-TMS ester) and (g) N-Ac-Gly. The y-axis (abundance) is scaled to the most abundant peak of this segment and the x-axis (retention time in minutes) is cropped to only show segment B as indicated in Figure S1.

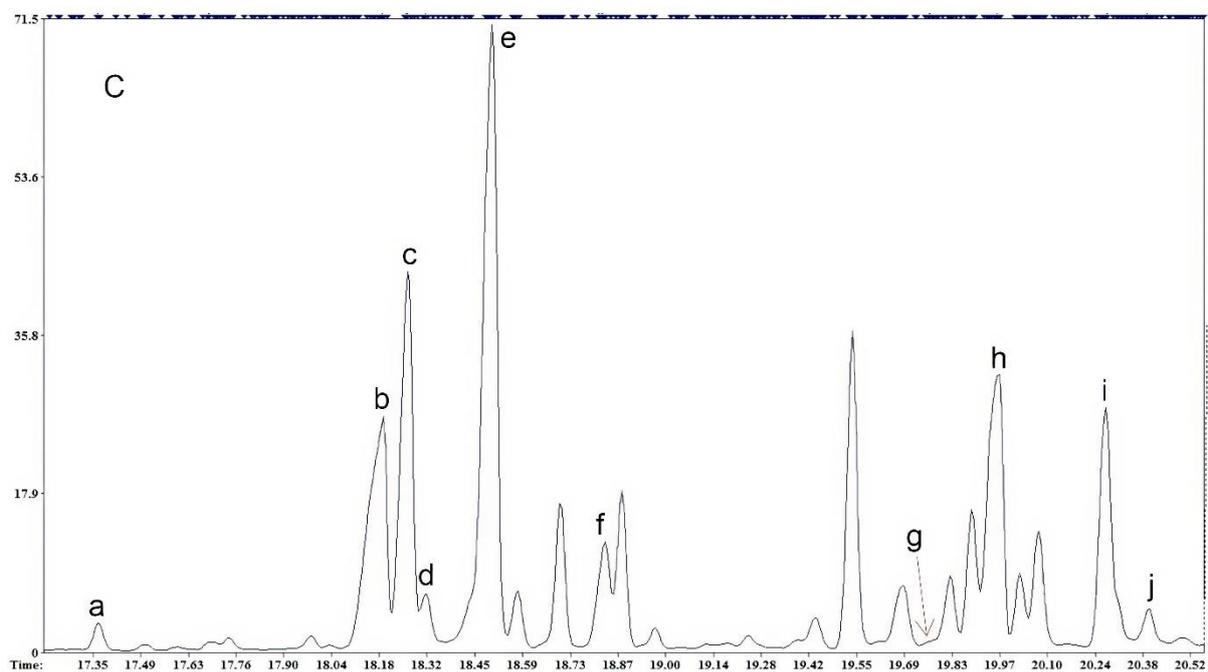


Figure S4: Segment C of Figure S1. The compound list is as follows: (a) N-Ac-Val (di-TMS ester), (b) N-Ac-Leu, (c) the internal standard, 3-phenylbutyric acid, (d) N-Ac-Ile, (e) N-hexanoyl-Gly, (f) N-isobutyryl-Val, (g) 5-hydroxy-5-methylhydantoin, (h) N-isobutyryl-Leu, (i) N-isobutyryl-Ile and (j) N-2-methylbutyryl-Val. The y-axis (abundance) is scaled to the most abundant peak of this segment and the x-axis (retention time in minutes) is cropped to only show segment C as indicated in Figure S1.

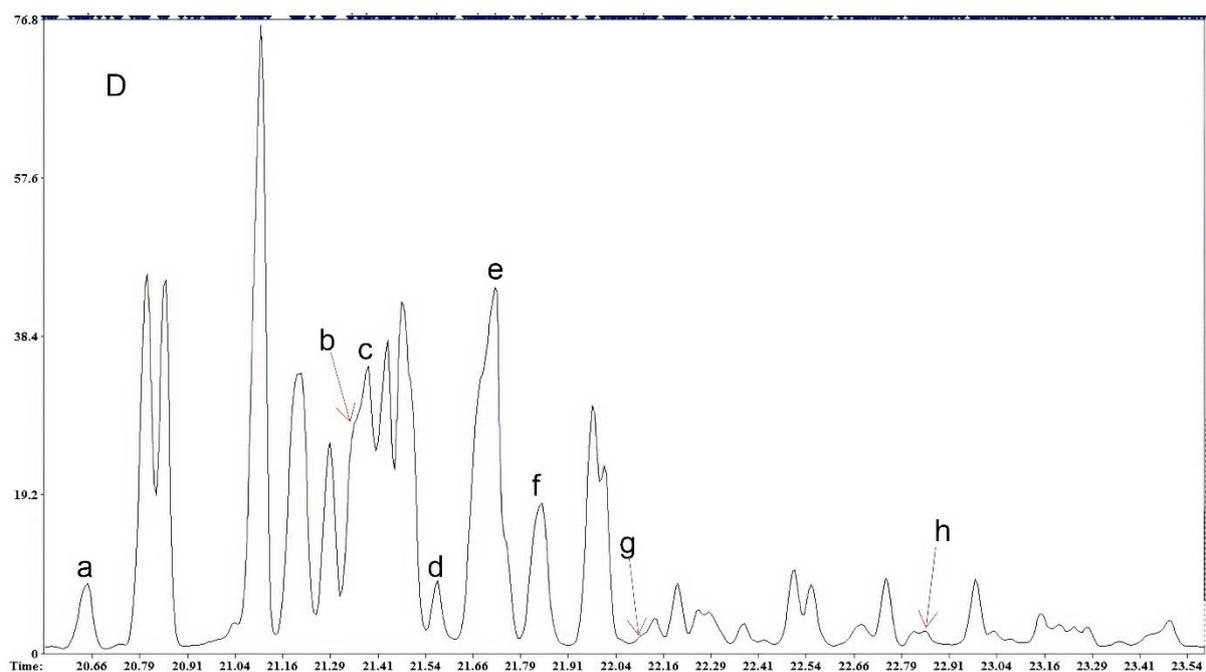


Figure S5: Segment D of Figure S1. The compound list is as follows: (a) N-isovaleryl-Val, (b) N-isovaleryl-Leu (mono-TMS ester), (c) N-2-methylbutyryl-Leu, (d) N-isovaleryl-Ile, (e) N-2-methylbutyryl-Ile, (f) N-isovaleryl-Leu (di-TMS ester), (g) 5-hydroxy-5-isopropylhydantoin and (h) N-lactyl-Ile. The y-axis (abundance) is scaled to the most abundant peak of this segment and the x-axis (retention time in minutes) is cropped to only show segment D as indicated in Figure S1.

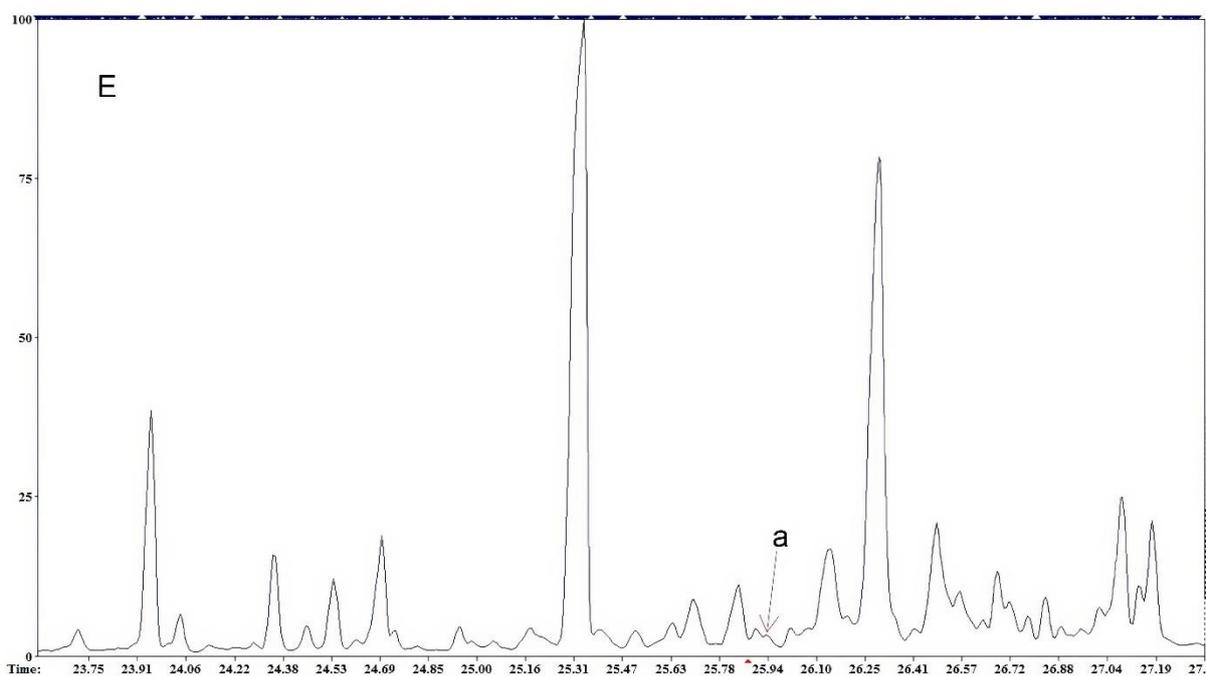


Figure S6: Segment E of Figure S1. Compound (a) indicates N-isovaleryl-Gln. The y-axis (abundance) is scaled to the most abundant peak of this segment and the x-axis (retention time in minutes) is cropped to only show segment E as indicated in Figure S1.

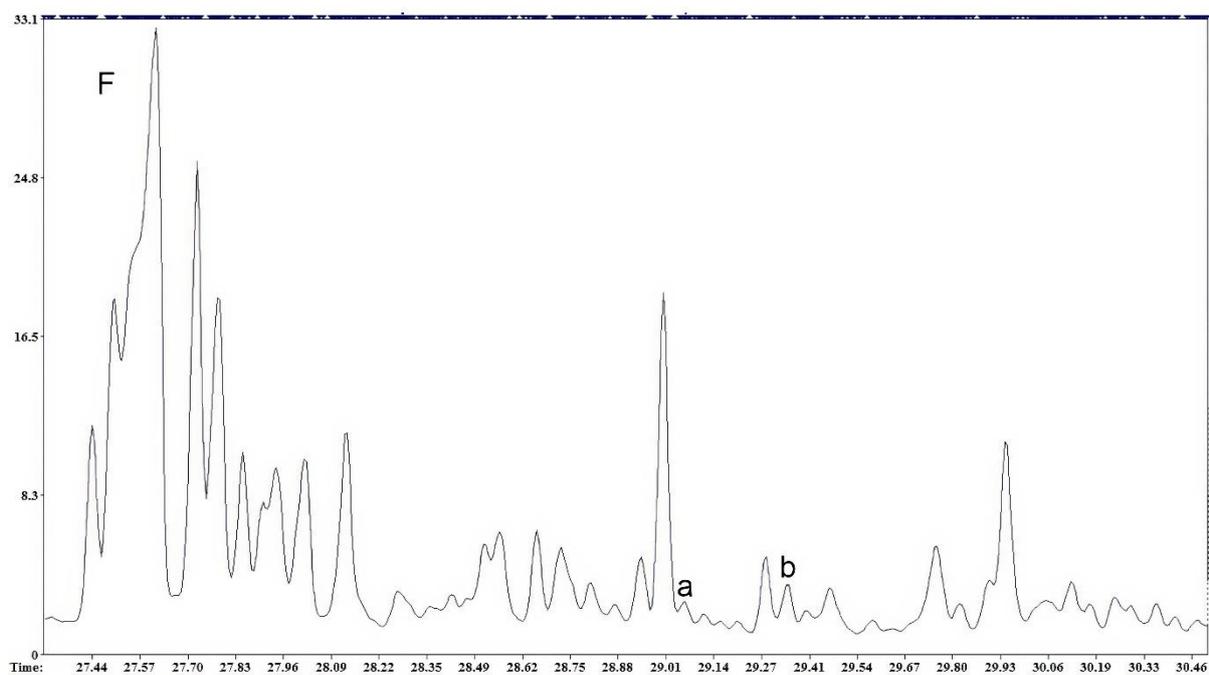


Figure S7: Segment F of Figure S1. The compound list is as follows: (a) N-2-methylbutyryl-Ile and (b) N-phenylacetyl-Gln. The y-axis (abundance) is scaled to the most abundant peak of this segment and the x-axis (retention time in minutes) is cropped to only show segment F as indicated in Figure S1.