**Supplementary Table Legends**

**Supplementary Table S1.** List of metabolites identified using the 2D-GC/ToF-MS platform. HMDB, PubChem, ChEBI, KEGG and METLIN identifiers are provided with the raw unprocessed peak abundance data. Derivatized metabolites are highlighted in yellow.

**Supplementary Table S2.** List of enriched pathways for the 2D-GC/ToF-MS –based quantified metabolites. P-values and Impact scores of the pathways are provided.

**Supplementary Table S3.** List of metabolites identified using the Orbitrap-MS platform. HMDB, PubChem, ChEBI, KEGG and METLIN identifiers are provided with the raw unprocessed peak abundance data. Derivatized metabolites are highlighted in yellow.

**Supplementary Table S4.** List of enriched pathways for the 1D-GC/Orbitrap-MS–based quantified metabolites. P-values and Impact scores of the pathways are provided.

**Supplementary Figure 1.** EI-MS spectra examples for (A) Glycerol-3TMS, (B) Urea-2TMS, obtained for 1D-GC-Orbitrap-MS and (C) Glycerol-3TMS, (D) Urea-2TMS, for 2D-GC-ToF-MS.