



Figure S1. Data analysis workflow.

All the standard mixtures and serum samples were prepared, derivatized, and analyzed. In brief, after TMS derivatization, each 1 μ L aliquot of the derivatized solution was injected in splitless mode into Agilent 7890B GC unit coupled to a Bench TOF-Select™ system (Markes International, Llantrisant, UK). Derivatization reaction aimed to increase the volatility of metabolites was then initiated by adding 25 μ L of pyridine and 50 μ L of the silylating agent BSTFA (with 1% and heated at 70°C for 1 h. Under a gentle stream of nitrogen, the excess of the derivatization agent and the pyridine were removed. The dried residue was re-dissolved in 0.5 mL of n-hexane. Each sample was vortex-mixed, after adding internal standard, and carefully transferred to the GC autosampler vials for subsequent GC-TOF-MS analysis.