### Text S3: Sample Preparation and 1H-NMR Spectroscopic Analysis

Heparin blood plasma samples (400 µL) were introduced into 5 mm NMR tubes with 200 µL of deuterated phosphate buffer solution (KH2PO4 with a final concentration of 0.2M). Deuterium was employed as locking substance. 24 hours urine samples (400 µL) were introduced into 5 mm NMR tubes with 200 µL of deuterated phosphate buffer solution (KH2PO4 with a final concentration of 0.2M, and containing 1 mM of sodium 3-(trimethylsilyl)-[2,2,3,3-2H4]-1-propionate (TSP). Metabolic profiles were measured on a Bruker Avance III 600 MHz spectrometer equipped with an inverse 5mm cryogenic probe at 300 K (Bruker Biospin, Rheinstetten, Germany). Urine samples were measured using a standard pulse sequence with water suppression during a relaxation delay (RD) of 4 s. Standard 1H-NMR one-dimensional pulse sequence with water suppression (RD=4s), Carr-Purcell-Meiboom-Gill (CPMG) spin-echo sequence with water suppression (RD=4s), and diffusion-edited sequence (RD=1s) where acquired for each plasma sample. For each one dimensional experiment 16 and 32 scans were collected using 98 K data points for urine and plasma samples, respectively. 1H-NMR spectra were processed using TOPSPIN (version 2.1, Bruker, Germany) software package prior to Fourier transformation. The acquired NMR spectra were manually phased and baseline corrected, and referenced to the chemical shift of the anomeric proton of α-glucose at δ 5.236 for plasma spectra and of TSP at δ 0.00 for urine. The assignment of the 1H-NMR resonances to specific metabolites was achieved by matching our in-house developed NMR database of pure compounds and using literature data [1,2]. Metabolite identification was confirmed by 2D 1H-1H COrrelation SpectroscopY (COSY) [3], 1H-1H TOtal Correlation SpectroscopY (TOCSY) [4] and 1H-13C Heteronuclear Single Quantum Correlation (HSQC) [5] NMR techniques.

Reference List

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