**Analysis protocol:**

*Instrument* – Metabolites were analyzed by NMR spectroscopy using a 600 MHz AVANCE III HD instrument (Bruker) equipped with a 5-mm TCI cryoprobe.

*Data acquisition*– Bruker’s default pulse programs pulse program of 1H-13C heteronuclear single quantum correlation (HSQC, hsqcetgpprsisp2.2 by Bruker nomenclature) was used. Corresponding acquisition parameters are in ‘6\_Acquisition and processing parameters\_UGA\_temp\_Oct2023\_drawdown.xlsx. Experiment details for individual samples are also in ‘1\_Study design\_UGA\_temp\_Oct2023\_drawdown.xlsx’. Experiments were conducted using TopSpin version 3.5 (Bruker).

*Data processing* – Raw Bruker spectra were processed by NMRPipe1 on NMRbox2. Detailed data processing parameters for individual NMR experiments are in ‘6\_Acquisition and processing parameters\_UGA\_temp\_Oct2023\_drawdown.xlsx. The NMRPipe processing scripts and processed .ft2 files are in ‘code’ and ‘ft’ in ‘Data\_analysis/Analysis/Inputs/Spectra/NMRpipe’, respectively.

*Downstream data analysis:* Peak intensity was extracted by rNMR version 1.11. Downstream analysis was conducted using MATLAB versions later R2023b (MathWorks). All the input files, processing steps and scripts, and the output files are available in folder ‘Data\_analysis’.

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