**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 programs of 1H-13C heteronuclear single quantum correlation (HSQC, hsqcetgpprsisp2.2 by Bruker nomenclature) and 1H-13C HSQC-total correlation spectroscopy (HSQC-TOCSY, hsqcdietgpsisp.2) were used. Acquisition parameters used are in ‘6\_Acquisition and processing parameters\_UGA\_temp\_Oct2023\_main.xlsx. Experimental details are also in ‘1\_Study design\_UGA\_temp\_Oct2023\_main.xlsx’. Experiments were conducted using TopSpin version 3.5 (Bruker).

*Data processing* – The raw Bruker spectra data were processed by NMRPipe1, except two spectra for compound annotation that were processed using TopSpin. Detailed data processing parameters are in ‘6\_Acquisition and processing parameters\_UGA\_temp\_Oct2023\_main.xlsx. The NMRPipe processing scripts and processed .ft2 files are in ‘Data\_analysis/Analysis/Inputs/Spectra/NMRpipe’.

*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 output files are available in folder ‘Data\_analysis’.

*1*Delaglio, F.; Grzesiek, S.; Vuister, G. W.; Zhu, G.; Pfeifer, J.; Bax, A., NMRPipe - a Multidimensional Spectral Processing System Based on Unix Pipes. J Biomol Nmr 1995, 6 (3), 277-293.