

## Description of Additional Supplementary Files

**Supplementary Data 1.** A list of all the metabolites measured and their technical details. The summary statistics are measured from log<sub>2</sub> transformed raw data.

**Supplementary Data 2.** The batch sample arrangement design represented as a plate format used in the study to embed intra-batch and inter-batch sample replicates. There are 8 rows and 11 columns per batch, samples marked with "\*" indicates intra-batch sample replicates and "\*\*\*" indicates inter-batch sample replicates.