

Description of Additional Supplementary Files

File name: Supplementary Data 1

Description: P PERMANOVA summary

File name: Supplementary Data 2

Description: Metabolites summary: statistical analysis, Qemistree classification and Mmvec ordination.

File name: Supplementary Data 3

Description: MASST results

File name: Supplementary Data 4

Description: Samples information

File name: Supplementary Data 5

Description: MASST job links in GNPS