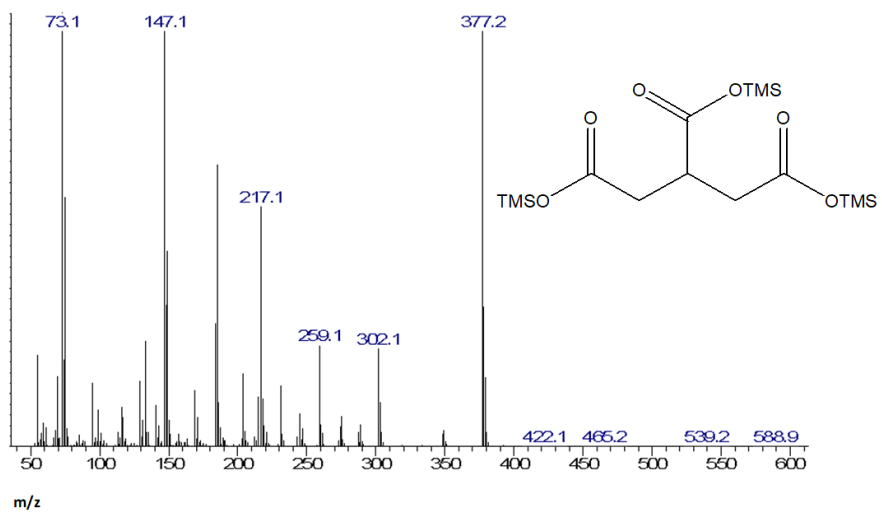


Supplemental Figure 1: Post derivatization structures of citric acid cycle metabolites under the study. TMS- Trimethylsilyl

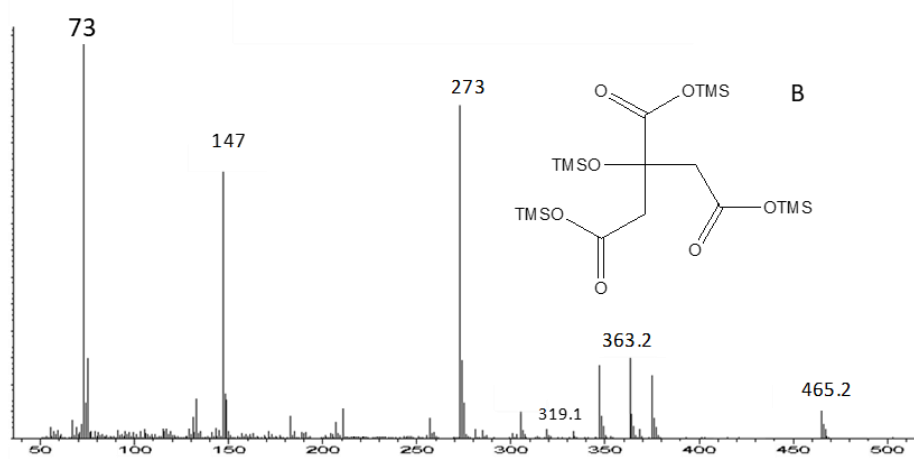
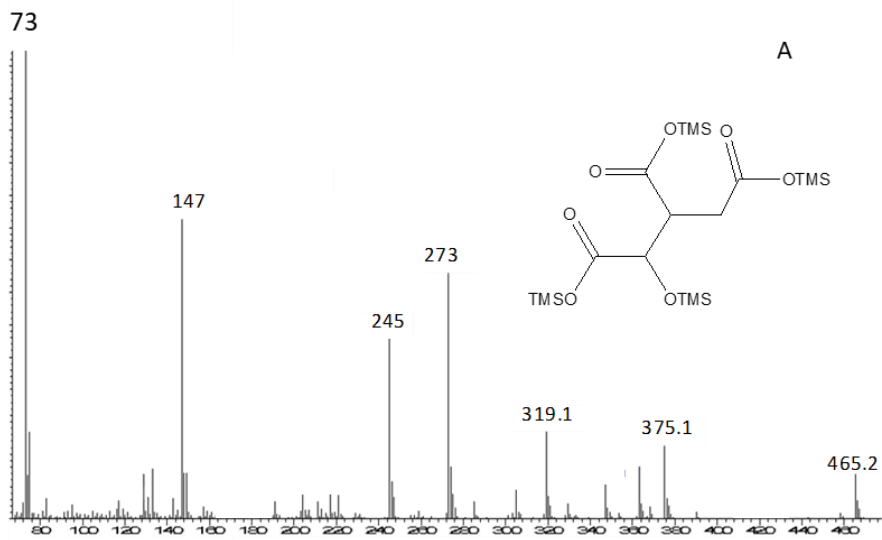
Analyte/Internal standard	RT	Target ions
Succinate/ Succinate d_6^*	7.22	m/z 247; 251
Fumarate/ Fumarate $^{13}C_4$	7.53	m/z 245; 249
Malate/ Malate $^{13}C_4$	8.8	m/z 233; 236
α -Ketoglutarate/ α - Ketoglutarate d_6^*	9.5	m/z 304; 308
Citrate/ Citrate $^{13}C_6$	11.4	m/z 273; 278
Aconitate/Tricarballic acid	10.8/10.7	m/z 229; 377
Isocitrate/Tricarballic acid	11.4/10.7	m/z 245; 377

*Deuterium labeling on acidic positions is lost during derivatization process.

Supplemental Table 1: Target ions and retention times for all analytes and internal standards



Supplemental figure 2: Tricarballic acid EI-MS spectrum



Supplemental figure 3: (A) isocitrate and (B) citrate EI-MS spectra. m/z 245 is specific to isocitrate

Supplemental Figure 4: Calculated HSI. NAFLD (n=22) and control (n=67). Statistical analysis performed by Prism 8 (GraphPad). * p<0.05

