

Supplementary Table 2 Mass Spectrometry characteristics of compounds monitored by targeted analysis through Liquid Chromatography - Tandem Mass Spectrometry (LC/MS/MS) in blood and urine samples collected over the study period.

| Compound | Precursor ion [M+H]⁺ <i>m/z</i> | Product ions [M+H]⁺ <i>m/z</i> |
|-----------------|---|--|
| TMAO | 76 | 58 |
| TMAO-d9 | 85 | 66 |
| Betaine | 118 | 59 |
| Carnitine | 162 | 103; 85; 60 |
| Choline | 104 | 60 |
| Creatinine | 114 | 44 |

TMAO: trimethylamine n-oxide; TMAO-d9: deuterium-labeled methyl d9-TMAO. *m/z*, mass-to-charge.