**Supplementary Table 2.** Summary of baseline reproducibility of candidate plasma metabolite biomarkers (n=17 patients).

|  |  |  |
| --- | --- | --- |
| **Metabolite** | **Pearson’s correlation coefficient** | **Mean coefficient of variation** |
| Asparagine | 0.934 | 0.19 |
| Citrulline | 0.999 | 0.14 |
| Glutamate | 0.896 | 0.18 |
| Histidine | 0.797 | 0.08 |
| Isoleucine | 0.404 | 0.12 |
| Leucine | 0.555 | 0.10 |
| Phenylalanine | 0.669 | 0.08 |
| Serine | 0.572 | 0.12 |
| Threonine | 0.714 | 0.16 |
| Tryptophan | 0.765 | 0.10 |
| Valine | 0.818 | 0.07 |
| C3 AC | 0.624 | 0.17 |
| C5 AC | 0.580 | 0.19 |
| C14:2-OH AC | 0.303 | 0.32 |
| C16 AC | 0.815 | 0.13 |
| C16:1-OH AC | 0.807 | 0.17 |
| C18 AC | 0.696 | 0.15 |
| C18:1 AC | 0.632 | 0.18 |
| C18:1-OH AC | 0.798 | 0.17 |
| lysoPC a C18:1 | 0.733 | 0.17 |
| lysoPC a C20:3 | 0.796 | 0.18 |
| lysoPC a C20:4 | 0.714 | 0.15 |
| PC aa C36:0 | 0.731 | 0.47 |
| PC ae C40:1 | 0.566 | 0.18 |
| PC ae C42:3 | 0.877 | 0.11 |
| PC ae C42:4 | 0.882 | 0.12 |

(a, acyl; aa, acyl-acyl; ae, acyl-alkyl; Cx:y, where x is the number of carbons in the fatty acid side chain; y is the number of double bonds in the fatty acid side chain; AC, acylcarnitine; DC, decarboxyl; M, methyl; OH, hydroxyl; PC, phosphatidylcholine)