Supplementary Material

**Identification of pre-frailty sub-phenotypes in elderly using metabolomics**

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# Supplementary Tables

**Table 1S:** Summary of identifications of serum metabolites.

1Identified compounds confirmed with authentic standards (level 1, (Sumner et al., 2007)), 2Putatively annotated compounds (level 2, (Sumner et al., 2007)), 3Putatively characterized compound (level 3, (Sumner et al., 2007)).

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| --- | --- | --- | --- | --- | --- |
| **Metabolic Pathway** | **Name** | **Variable label** | **Annotation** | **Retention time (min)** | **Measured mass (*m*/*z*)** |
| Amino acid metabolism | Glutamine1 | M151T50 | [M+Na-H2O]+ | 0.83 | 151.04774 |
| 2,4 diaminobutyric acid1 | M101T50 | [M+H-H2O]+ | 0.84 | 101.07092 |
| Threonine1 | M120T51 | [M+H]+ | 0.85 | 120.06543 |
|  | M74T51 | [M+H-CH2O2]+ | 0.85 | 74.06007 |
| Phenylalanine1 | M131T359 | [M+H-H2O-NH3]+ | 5.99 | 131.04920 |
| Pipecolic acid2 | M130T70 | [M+H]+ | 1.16 | 130.08639 |
| Proline1 | M116T57 | [M+H]+ | 0.95 | 116.0703 |
| Amino-octanoic acid3 | M160T491 | C8H18O2N+ | 8.19 | 160.13318 |
| Glutamic acid1 | M130T50 | [M+H-H2O]+ | 0.84 | 130.04982 |
| Alanine1 | M90T51 | [M+H]+ | 0.84 | 90.05485 |
| Carbohydrate metabolism | Mannose1 | M198T53 | [M+NH4]+ | 0.88 | 198.09741 |
| Fructose1 | M383T52 | [2M+Na]+ | 0.87 | 383.11607 |
|  | M384T52 | 13C[2M+Na]+ | 0.87 | 384.11950 |
|  | M443T52 | [2M+2Na+K-2H]+ | 0.87 | 443.07214 |
| Lactose1 | M325T52 | [M+Na-NaOH]+ | 0.87 | 325.11298 |
| Deoxyglucose1 | M187T58 | [M+H]+ | 0.98 | 187.05772 |
| Lipid metabolism | Butyrylcarnitine1 | M232T412 | [M+H]+ | 6.87 | 232.15438 |
| Isovalerylcarnitine1 | M246T473 | [M+H]+ | 7.88 | 246.17003 |
| LysoPE(16:0)1 | M454T904 | [M+H]+ | 15.06 | 454.29240 |
| lysoPE(18:1)2 | M480T927 | [M+H]+ | 15.45 | 480.30998 |
| lysoPE(18:2)2 | M478T874 | [M+H]+ | 14.57 | 478.29360 |
| PG(26:1)3 | M636T625 | C32H61O10P+ | 10.41 | 636.39859 |
| Peptides | N-(2-Hydroxypropyl)-valine2 | M176T61 | [M+H]+ | 1.01 | 176.12791 |
| Gly-Phe1 | M223T435 | [M+H]+ | 7.26 | 223.10662 |
| Pyr-Glu-Ala3 | M351T58 | C13H20N4NaO6+ | 0.97 | 351.12618 |
| Food metabolites | Dimethyloxazole2 | M98T371 | [M+H]+ | 6.18 | 98.06028 |
| 2,3-dihydromethylpyrrole3 | M84T71 | C5H9N | 1.18 | 84.08110 |
| trigoneline1 | M138T56 | [M+H]+ | 0.94 | 138.05439 |
| Dihydroxyphenyl acetic acid3 | M169T41 | C8H8O4+ | 0.69 | 169.04605 |
| Unknown | Unknown | M146T41 | C3H8NO4Mg+ | 0.68 | 146.02986 |
| Unknown | M610T45 |  | 0.75 | 609.96090 |

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