Table 2. Unidirectional trends of changes in the intensities (peak-AUC) of identified metabolites before and after bariatric surgery, metabolites in bold have previously been associated with CVR.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Metabolite**  **(Ionization-mode)** | **MzMed** | **RtMed** | **p-value\*\* PRE-POST** | **p-value\*\* PRE-FU** | **Ratio PRE-POST** | **Ratio PRE-FU** | |
|  |  | decreasing trend |  |  | | |
| **Alanine (+)** | 90.0556 | 12.20 | <0.001 | 0.019 | 0.8 | 0.85 | |
| **Choline (+)** | 104.1076 | 10.06 | <0.001 | 0.003 | 0.74 | 0.79 | |
| **Leucine/isoleucine° (+)** | 132.1022 | 9.45 | 0.003 | <0.001 | 0.87 | 0.77 | |
| Lysine (-) | 145.0968 | 13.02 | 0.036 | <0.001 | 0.91 | 0.88 | |
| Oxovaleric acid (-) | 115.0384 | 9.90 | <0.001 | <0.001 | 0.81 | 0.74 | |
| Pentoses (-) | 149.0441 | 9.96 | 0.127 | <0.001 | 0.93 | 0.78 | |
| **Phenylalanine (+)** | 166.0865 | 9.74 | 0.003 | <0.001 | 0.88 | 0.83 | |
| Tyrosine (-) | 180.0658 | 11.28 | <0.001 | <0.001 | 0.79 | 0.73 | |
| Uridine (-) | 243.0617 | 7.20 | 0.004 | 0.006 | 0.82 | 0.81 | |
| **Valine° (-)** | 116.0700 | 10.19 | <0.001 | <0.001 | 0.82 | 0.75 | |
|  |  | increasing trend |  |  | | |
| Glutamine° (+) | 147.0767 | 13.63 | <0.001 | 0.003 | 1.17 | 1.2 | |
| Glycine° (+) | 76.0400 | 9.60 | <0.001 | <0.001 | 1.24 | 1.35 | |
| Hydroxydecanoic acid (-) | 187.1329 | 9.45 | <0.001 | <0.001 | 1.59 | 2.68 | |
| **Indoxyl sulphate (-)** | 212.0013 | 9.13 | 0.067 | <0.001 | 1.35 | 2.38 | |
| PC C40:7 (+) | 832.5865 | 5.14 | 0.641 | <0.001 | 1.04 | 1.4 | |
| **Trimethylamin-N-oxid (+)** | 76.0764 | 11.88 | 0.022 | <0.001 | 1.99 | 2.59 | |

\*\* unadjusted p-values from paired t-test, ° metabolites identified with targeted approach

Table 3. Bidirectional trends of changes in the intensities (peak-AUC) of identified metabolites before and after bariatric surgery, metabolites in bold have previously been associated with CVR.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Metabolite\*\*\***  **(Ionization-mode)** | **MzMed** | **RtMed** | **p-value\*\* PRE-POST** | **p-value\*\* PRE-FU** | **Ratio PRE-POST** | **Ratio PRE-FU** | |
|  |  | V-pattern |  |  |  |  |
| Creatine (+) | 132.0771 | 12.19 | <0.001 | <0.001 | 0.66 | 0.72 | |
| LysoPC C16:1 (+) | 494.3249 | 4.83 | 0.077 | 0.288 | 0.85 | 1.09 | |
| LysoPC C18:2 (+) | 520.3407 | 5.13 | <0.001 | 0.863 | 0.68 | 1.01 | |
| **Ornithine (-)** | 131.0815 | 12.54 | 0.004 | 0.019 | 0.83 | 1.11 | |
| PC C34:3 (+) | 756.5550 | 5.27 | <0.001 | 0.370 | 0.66 | 0.95 | |
| PC C36:5 (+) | 780.5550 | 5.01 | <0.001 | 0.006 | 0.67 | 0.81 | |
| PC C36:6 (+) | 778.5389 | 4.61 | <0.001 | 0.809 | 0.48 | 0.98 | |
| Sarcosine (-) | 88.0386 | 11.27 | <0.001 | <0.001 | 0.78 | 0.86 | |
| Tryptophan (+) | 205.0973 | 9.83 | <0.001 | <0.001 | 0.74 | 0.81 | |
| Uracil (+) | 113.0351 | 6.98 | <0.001 | <0.001 | 0.75 | 0.78 | |
|  |  | Ʌ-pattern |  |  |  | | |
| Acetylglycine (-) | 116.0337 | 12.97 | <0.001 | <0.001 | 2.78 | 2.05 | |
| Arginine (+) | 175.1193 | 12.15 | 0.620 | 0.233 | 0.97 | 1.05 | |
| Carnitine (+) | 162.1127 | 10.88 | 0.004 | 0.515 | 1.19 | 1.03 | |
| Hydroxyisobutyric acid (-)# | 103.0387 | 12.10 | <0.001 | <0.001 | 3.3 | 0.71 | |
| Leu Pro (+) # | 229.1548 | 9.19 | <0.001 | 0.180 | 1.64 | 0.9 | |
| LysoPE C20:4 (+) | 502.2936 | 8.27 | 0.022 | 0.227 | 1.16 | 1.09 | |
| Pantothenic acid (-) | 218.1025 | 12.69 | 0.001 | 0.270 | 1.52 | 1.14 | |
| PC C38:6 (+) | 806.5705 | 5.21 | <0.001 | 0.020 | 1.31 | 1.15 | |
| Pyroglutamic acid (-) | 128.0337 | 12.89 | 0.002 | 0.038 | 1.18 | 1.1 | |
| Threonine (+) | 120.0660 | 13.11 | 0.602 | <0.001 | 1.04 | 0.79 | |

\*\* unadjusted p-values from paired t-test, # standards available for all „identified metabolites“, except for hydroxydecanoic acid (annotated) and Leu Pro (Metlin annotated)