A picture containing text

Description automatically generated

**Figure S1**: **Boxplot of Total Bilirubin across all the groups with p-values**. Showing statistically significant higher values of Total Bilirubin in PDAC groups RPC, LAPC and MPC compared to CP using Wilcoxon Rank Sum test. Higher values of bilirubin may be due by bile obstruction, which might cause damage to the liver. CP: Chronic pancreatitis; RPC: Resectable Pancreatic Ductal Adenocarcinoma; LAPC: Locally Advanced Pancreatic Ductal Adenocarcinoma; MPC: Metastatic Pancreatic Ductal Adenocarcinoma

A picture containing light, traffic, dark

Description automatically generated

**Figure S2**: **Correlation of Glucose and Inflammatory markers.** GlycB has a positive correlation with glucose. Elevated glucose levels detected in the blood could be because of chronic inflammation on decreasing insulin secretion and sensitivity. Black-square boxes represent PDAC patients with T2DM. There was no direct correlation of diabetes with the markers. The outlier could be sample collected from a patient with high blood sugar levels after feeding. T2DM: Type 2 Diabetes, PDAC: Pancreatic Ductal Adenocarcinoma.

**Table S1.** List of the quantified signal and their relative assignment and multiplicity.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Metabolite** | **Assignment (multiplicity)** | **matrix** |  | **Metabolite** | **Assignment (multiplicity)** | **matrix** |
| Formate | 8.45 (s) | serum |  | cholesterol-derivated 1 | 0.64 (s) | lipid extracts |
| Unknown signal at 8.12 ppm | 8.12 (d) | serum |  | cholesterol-derivated 2 | 0.65 (s) | lipid extracts |
| Unknown signal at 8.07 ppm | 8.07 (d) | serum |  | cholesterol-derivated 3 | 0.66 (s) | lipid extracts |
| Phenylalanine | 7.42 (m) | serum |  | cholesterol-derivated 4 | 0.66 (s) | lipid extracts |
| Tyrosine | 7.19 (m) | serum |  | cholesterol-derivated 5 | 0.67 (s) | lipid extracts |
| Unknown signal at 7.14 ppm | 7.14 (m) | serum |  | free cholesterol | 0.68 (s) | lipid extracts |
| Histidine | 7.05 (d) | serum |  | esterified cholesterol | 0.68 (s) | lipid extracts |
| Glucose | 5.23 (d) | serum |  | cholesterol-derivated 6 | 0.69 (s) | lipid extracts |
| Mannose | 5.18 (d) | serum |  | cholesterol-derivated 7 | 0.70 (s) | lipid extracts |
| Unknown signal at 5.15 ppm | 5.15 (d) | serum |  | cholesterol-derivated 8 | 0.70 (s) | lipid extracts |
| Unknown signal at 5.09 ppm | 5.09 (d) | serum |  | cholesterol-derivated 9 | 0.71 (s) | lipid extracts |
| Unknown signal at 5.01 ppm | 5.01 (d) | serum |  | saturated and omega-9 fatty acid | 0.87 (t) | lipid extracts |
| Ascorbate | 4.50 (d) | serum |  | omega-7 fatty acid | 0.87 (t) | lipid extracts |
| Threonine | 4.24 (m) | serum |  | omega-6 fatty acid | 0.88 (t) | lipid extracts |
| Lactate | 4.11 (q) | serum |  | Unknown signal at 0.91 ppm | 0.98 (d) | lipid extracts |
| Creatinine | 4.05 (s) | serum |  | omega-3 fatty acid | 0.99 (t) | lipid extracts |
| Creatine | 3.92 (s) | serum |  | monounsaturate fatty acid | 2.01 (q) | lipid extracts |
| Glycine | 3.55 (s) | serum |  | polyunsaturate fatty acid 1 (except linoleic) | 2.80 (t) | lipid extracts |
| Methanol | 3.35 (s) | serum |  | polyunsaturate fatty acid 2 (except linoleic) | 2.84 (d) | lipid extracts |
| Unknown signal at 2.55 ppm | 2.55 (s) | serum |  | linoleic acid | 2.76 (t) | lipid extracts |
| Citrate | 2.53 (d) | serum |  | phosphatidylcholine | 3.20 (s) | lipid extracts |
| Glutamine | 2.45 (m) | serum |  | sphingomyelin | 3.19 (s) | lipid extracts |
| Pyruvate | 2.36 (s) | serum |  | triglyceride | 5.26 (m) | lipid extracts |
| Glutamate | 2.53 (m) | serum |  | glycerophospholipid | 4.45 (q) | lipid extracts |
| Acetoacetate | 2.22 (s) | serum |  |  |  |  |
| Acetate | 1.91 (s) | serum |  |  |  |  |
| Alanine | 1.47 (d) | serum |  |  |  |  |
| Unknown signal at 1.45 ppm | 1.45 (d) | serum |  |  |  |  |
| Unknown signal at 1.43 ppm | 1.43 (d) | serum |  |  |  |  |
| 3-Hydroxybutyrate | 1.19 (d) | serum |  |  |  |  |
| Ethanol | 1.17 (t) | serum |  |  |  |  |
| Unknown signal at 1.16 ppm | 1.16 (d) | serum |  |  |  |  |
| Unknown signal at 1.14 ppm | 1.14 (d) | serum |  |  |  |  |
| Unknown signal at 1.11 ppm | 1.11 (d) | serum |  |  |  |  |
| Unknown signal at 1.06 ppm | 1.06 (d) | serum |  |  |  |  |
| Valine | 1.04 (d) | serum |  |  |  |  |
| Isoleucine | 1.00 (d) | serum |  |  |  |  |
| Leucine | 0.95 (dd) | serum |  |  |  |  |
| 2-Hydroxybutyrate | 0.89 (t) | serum |  |  |  |  |
| Protein NH | 10.00-6.00 | serum |  |  |  |  |
| Unsaturated lipid -CH=CH- | 5.50-5.10 | serum |  |  |  |  |
| Lipid alpha-CH2 | 2.25-2.15 | serum |  |  |  |  |
| Cholesterol | 0.70-0.60 | serum |  |  |  |  |
| Lipid =CH-CH2-CH= | 2.85-2.65 | serum |  |  |  |  |
| Glycorol phospholipid | 4.08-4.03 | serum |  |  |  |  |
| Phospholipid | 3.68-3.62 | serum |  |  |  |  |
| Lipid beta-CH2 | 1.65-1.40 | serum |  |  |  |  |
| Lipid CH2 | 1.40-1.10 | serum |  |  |  |  |
| Lipid CH3 | 1.10-1.08 | serum |  |  |  |  |
| GlycB | 2.07 (m) | serum |  |  |  |  |
| GlycA | 2.03 (m) | serum |  |  |  |  |

**Table S2:** Selectedmetabolites ratios and their catalysing enzymes

|  |  |
| --- | --- |
| **Ratio** | **Catalysing enzymes** |
| Glucose/Lactate | Phosphofructokinase |
| Pyruvate/Lactate | Lactate dehydrogenase |
| Threonine/Glycine | Threonine dehydrogenase  2-amino-3-ketobutyrate coenzyme A ligase |
| Glutamine/Glutamate | Glutamine synthetase |
| 3-hydroxybutyrate/acetoacetate | 3-hydroxybutyrate dehydrogenase |
| Glutamate/Alanine | Alanine aminotransferase |

**Table S3:** Haematological parameters of the Pancreatic Ductal Adenocarcinoma and Chronic Pancreatitis patient groups.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Feature** | **CP**  **median [IQR]** | **RPC**  **median [IQR]** | **LAPC**  **median [IQR]** | **MPC**  **median [IQR]** | **p-val** | **FDR** |
| Haematocrit | 0.385 [0.282 0.455] | 0.316 [0.281 0.367] | 0.303 [0.244 0.325] | 0.339 [0.304 0.373] | 0.482 | 0.620 |
| white.cell.count (/L^9) | 6.83 [6.153 8.182] | 8.89 [6.91 12.4] | 10.845 [7.927 11.037] | 9.905 [4.225 17.31] | 0.484 | 0.620 |
| Haemaglobin (g/DL) | 12.7 [9.6 14.6] | 10.25 [9.475 11.525] | 9.4 [7.825 10.775] | 10.95 [10 11.6] | 0.507 | 0.620 |
| Platelet.count (/L^9) | 245 [222.75 339.25] | 372.5 [313 502.75] | 436.5 [324.25 497] | 358 [317.75 405.25] | 0.206 | 0.594 |
| Prothrombin.time | 12.1 [11.675 12.9] | 13.2 [12.5 15.2] | 14.35 [13.025 14.525] | 14.2 [13.525 16.05] | 0.151 | 0.594 |
| INR | 0.935 [0.927 0.975] | 1.08 [1 1.175] | 1.165 [1.048 1.183] | 1.165 [1.122 1.317] | 0.038 | 0.414 |
| MCV (fL) | 92.25 [88.525 93.275] | 93 [88 98.3] | 89.45 [87.675 91.675] | 91.25 [86.75 95.15] | 0.647 | 0.684 |
| MCH (pg) | 30.05 [28.25 31.325] | 30.2 [28.9 32.5] | 29.95 [28.825 30.825] | 28.5 [27.85 29.2] | 0.260 | 0.594 |
| MCHC (g/dl) | 32.3 [31.75 33.15] | 33.4 [32.2 33.8] | 33.1 [31.725 33.575] | 31.05 [30.8 31.775] | 0.312 | 0.594 |
| MPV (fL) | 10.3 [9.2 10.5] | 10.5 [9.6 10.9] | 10.4 [9.675 11.2] | 10.9 [10.575 11.225] | 0.324 | 0.594 |
| Red.cell.count.(/L^12) | 4.09 [3.018 4.878] | 3.49 [2.99 3.83] | 3.325 [2.538 3.852] | 3.77 [3.425 4.095] | 0.684 | 0.684 |

**CP: chronic pancreatitis; RPC: Resectable Pancreatic Ductal Adenocarcinoma; LAPC: Locally Advanced Pancreatic Ductal Adenocarcinoma; MPC: Metastatic Pancreatic Ductal Adenocarcinoma**

**Table S4:** Blood chemistry of the Pancreatic Ductal Adenocarcinoma and Chronic Pancreatitis patient groups.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Features** | **CP**  **median [IQR]** | **RPC**  **median [IQR]** | **LAPC**  **median [IQR]** | **MPC**  **median [IQR]** | **p-val** | **FDR** |
| Sodium.(mmol/L) | 138 [135.5 139.75] | 137 [135 140] | 135.5 [129.5 137.5] | 139.5 [138.5 141] | 0.295 | 0.889 |
| Potassium (mmol/L) | 4.05 [3.7 4.4] | 3.7 [3.4 4.1] | 3.55 [3.275 4.075] | 3.7 [3.125 4.3] | 0.659 | 0.889 |
| Chloride.(mmol/L) | 97.5 [97 101.75] | 96 [93 97] | 93.5 [89.75 96.5] | 90.5 [88.75 93] | 0.127 | 0.889 |
| Bicarbonate.(mmol/L) | 19.5 [18.25 20.75] | 23 [17 25] | 20 [19.75 21.5] | 24.5 [18.5 30.25] | 0.800 | 0.889 |
| Anion.gap..(mmol/L) | 24.5 [20.75 26.75] | 26 [19 30] | 23 [22 26.25] | 29.5 [25.75 33] | 0.445 | 0.889 |
| Calcium (mmol/L) | 2.26 [2.198 2.382] | 2.2 [2.11 2.31] | 2.105 [1.978 2.235] | 2.135 [2.128 2.148] | 0.403 | 0.889 |
| Magnesium.(mmol/L) | 0.865 [0.83 0.885] | 0.79 [0.68 0.9] | 0.77 [0.682 0.885] | 0.78 [0.72 1.16] | 0.800 | 0.889 |
| Inorganic.Phosphate.(mmol/L) | 1.18 [1.13 1.32] | 1.06 [0.96 1.2] | 1.085 [0.995 1.278] | 1.14 [1.098 1.367] | 0.477 | 0.889 |
| Urea..(mmol/L) | 4 [3.45 5.45] | 4 [2.2 5.5] | 3.5 [2.075 7.125] | 4.35 [3.05 6.325] | 0.945 | 0.645 |
| Creatinine..(µmol/L) | 90 [64.25 130] | 71 [58 95] | 64.5 [48 79.75] | 76.5 [72.75 80.25] | 0.585 | 0.889 |
|  |  |  |  |  |  |  |

**CP: chronic pancreatitis; RPC: Resectable Pancreatic Ductal Adenocarcinoma; LAPC: Locally Advanced Pancreatic Ductal Adenocarcinoma; MPC: Metastatic Pancreatic Ductal Adenocarcinoma**

**Table S5:** Correlation of concentration of metabolites with the stages of Pancreatic Ductal Adenocarcinoma

|  |  |  |  |
| --- | --- | --- | --- |
| **Feature** | **rho** | **p-val** | **FDR** |
| Formate | 0.22 | 0.151 | 0.513 |
| Unknown signal at 8.12 ppm | -0.01 | 0.941 | 0.995 |
| Unknown signal at 8.07 ppm | 0.3 | 0.043 | 0.235 |
| Phenylalanine | 0.32 | 0.030 | 0.235 |
| Tyrosine | 0.01 | 0.960 | 0.995 |
| Unknown signal at 7.14 ppm | 0.07 | 0.632 | 0.849 |
| Histidine | -0.03 | 0.841 | 0.933 |
| Glucose | 0.13 | 0.406 | 0.767 |
| Mannose | 0.2 | 0.181 | 0.543 |
| Unknown signal at 5.15 ppm | 0.18 | 0.232 | 0.564 |
| Unknown signal at 5.09 ppm | 0.05 | 0.727 | 0.905 |
| Unknown signal at 5.01 ppm | 0.12 | 0.439 | 0.793 |
| Ascorbate | -0.47 | 0.001 | 0.021 |
| Threonine | 0.16 | 0.282 | 0.600 |
| Lactate | 0.5 | <0.001 | 0.012 |
| Creatinine | -0.18 | 0.248 | 0.574 |
| Creatine | 0.08 | 0.582 | 0.811 |
| Glycine | 0.52 | <0.001 | 0.012 |
| Methanol | -0.19 | 0.202 | 0.543 |
| Unknown signal at 2.55 ppm | -0.09 | 0.542 | 0.811 |
| Citrate | 0 | 0.997 | 0.997 |
| Glutamine | -0.11 | 0.482 | 0.793 |
| Pyruvate | 0.28 | 0.060 | 0.278 |
| Glutamate | 0.24 | 0.115 | 0.450 |
| Acetoacetate | 0.1 | 0.529 | 0.811 |
| Acetate | 0.19 | 0.200 | 0.543 |
| Alanine | -0.03 | 0.822 | 0.932 |
| Unknown signal at 1.45 ppm | 0.32 | 0.032 | 0.235 |
| Unknown signal at 1.43 ppm | 0.18 | 0.226 | 0.564 |
| 3-Hydroxybutyrate | 0.11 | 0.467 | 0.793 |
| Ethanol | 0.04 | 0.804 | 0.932 |
| Unknown signal at 1.16 ppm | 0.15 | 0.339 | 0.692 |
| Unknown signal at 1.14 ppm | -0.31 | 0.035 | 0.235 |
| Unknown signal at 1.11 ppm | 0.31 | 0.041 | 0.235 |
| Unknown signal at 1.06 ppm | 0.04 | 0.800 | 0.932 |
| Valine | -0.2 | 0.182 | 0.543 |
| Isoleucine | 0.06 | 0.702 | 0.895 |
| Leucine | -0.26 | 0.083 | 0.354 |
| 2-Hydroxybutyrate | 0.3 | 0.046 | 0.235 |
| Protein NH | -0.42 | 0.005 | 0.058 |
| Unsaturated lipid -CH=CH- | -0.08 | 0.589 | 0.811 |
| Lipid alpha-CH2 | 0.17 | 0.271 | 0.600 |
| Cholesterol | 0.02 | 0.912 | 0.989 |
| Lipid =CH-CH2-CH= | -0.13 | 0.402 | 0.767 |
| Glycorol phospholipid | 0.07 | 0.658 | 0.861 |
| Phospholipid | 0 | 0.976 | 0.995 |
| Lipid beta-CH2 | -0.09 | 0.561 | 0.811 |
| Lipid CH2 | 0.05 | 0.755 | 0.916 |
| Lipid CH3 | -0.1 | 0.500 | 0.796 |
| GlycB | 0.23 | 0.129 | 0.471 |
| GlycA | 0.11 | 0.453 | 0.793 |

**Rho: spearman’s correlation coefficient measures the strength of association between two variables; FDR: false discovery rate**

**Table S6:** Correlation of concentration of lipid extracts with the stages of Pancreatic Ductal Adenocarcinoma

|  |  |  |  |
| --- | --- | --- | --- |
| **Features** | **rho** | **p-val** | **FDR** |
| cholesterol-derivated 1 | 0.32 | 0.047 | 0.154 |
| cholesterol-derivated 2 | 0.37 | 0.018 | 0.089 |
| cholesterol-derivated 3 | 0.24 | 0.133 | 0.195 |
| cholesterol-derivated 4 | 0.37 | 0.019 | 0.089 |
| cholesterol-derivated 5 | -0.29 | 0.065 | 0.154 |
| free cholesterol | 0.28 | 0.084 | 0.159 |
| esterified cholesterol | 0.09 | 0.587 | 0.587 |
| cholesterol-derivated 6 | 0.38 | 0.016 | 0.089 |
| cholesterol-derivated 7 | -0.16 | 0.313 | 0.327 |
| cholesterol-derivated 8 | 0.38 | 0.014 | 0.089 |
| cholesterol-derivated 9 | -0.33 | 0.037 | 0.148 |
| saturated and omega-9 fatty acid | 0.3 | 0.062 | 0.154 |
| omega-7 fatty acid | 0.37 | 0.017 | 0.089 |
| omega-6 fatty acid | 0.24 | 0.138 | 0.195 |
| Unknown signal at 0.91 ppm | -0.29 | 0.071 | 0.154 |
| omega-3 fatty acid | 0.27 | 0.086 | 0.159 |
| monounsaturate fatty acid | 0.26 | 0.110 | 0.180 |
| polyunsaturate fatty acid 1 (except linoleate) | 0.18 | 0.269 | 0.293 |
| polyunsaturate fatty acid 2 (except linoleate) | 0.23 | 0.149 | 0.199 |
| Linoleate | 0.21 | 0.194 | 0.233 |
| Phosphatidylcholine | 0.2 | 0.206 | 0.235 |
| Sphingomyelin | 0.3 | 0.065 | 0.154 |
| Triglyceride | 0.21 | 0.189 | 0.233 |
| Glycerophospholipid | 0.25 | 0.112 | 0.180 |

**Rho: spearman’s correlation coefficient measures the strength of association between two variables; FDR: false discovery rate**

**Table S7:** Correlation of metabolites ratios with the stages of Pancreatic Ductal Adenocarcinoma.

|  |  |  |  |
| --- | --- | --- | --- |
| **Feature** | **rho** | **p-val** | **FDR** |
| Glucose/Lactate | -0.19 | 0.212 | 0.424 |
| Pyruvate/Lactate | -0.14 | 0.360 | 0.599 |
| Threonine/Glycine | -0.09 | 0.540 | 0.674 |
| Glutamine/Glutamate | -0.26 | 0.089 | 0.222 |
| 3-Hydroxybutyrate/Acetoacetate | -0.05 | 0.767 | 0.767 |
| Glutamate/Alanine | 0.27 | 0.073 | 0.222 |

**Rho: spearman’s correlation coefficient measures the strength of association between two variables; FDR: false discovery rate**

**Table S8:** Correlation of concentration of lipoproteins with the stages of Pancreatic Ductal Adenocarcinoma

|  |  |  |  |
| --- | --- | --- | --- |
| **Feature** | **rho** | **p-value** | **FDR** |
| VLDL.C (nmol/L) | -0.07 | 0.667 | 0.754 |
| IDL.C (nmol/L) | 0.32 | 0.031 | 0.089 |
| LDL.C (nmol/L) | 0.22 | 0.151 | 0.230 |
| HDL.C (nmol/L) | -0.38 | 0.011 | 0.046 |
| VLDL.TG (nmol/L) | -0.03 | 0.840 | 0.910 |
| IDL.TG (nmol/L) | 0.28 | 0.060 | 0.139 |
| LDL.TG (nmol/L) | 0.3 | 0.043 | 0.112 |
| HDL.TG (nmol/L) | -0.08 | 0.607 | 0.717 |
| VLDL.P (nmol/L) | 0.01 | 0.964 | 0.964 |
| Large.VLDL.P.(nmol/L) | -0.13 | 0.404 | 0.500 |
| Medium.VLDL.P (nmol./L) | -0.23 | 0.121 | 0.211 |
| Small.VLDL.P.(nmol/L) | 0.02 | 0.916 | 0.953 |
| LDL.P (nmol/L) | 0.26 | 0.080 | 0.161 |
| Large.LDL.P.(nmol/L) | 0.21 | 0.174 | 0.251 |
| Medium.LDL.P.(nmol/L) | 0.28 | 0.064 | 0.139 |
| Small.LDL.P (nmol/L) | 0.15 | 0.333 | 0.450 |
| HDL.P (mol/L) | -0.39 | 0.008 | 0.046 |
| Large.HDL.P (mol/L) | -0.35 | 0.019 | 0.072 |
| Medium.HDL.P.(mol/L) | -0.39 | 0.008 | 0.046 |
| Small.HDL.P.(mol/L) | -0.39 | 0.009 | 0.046 |
| VLDL.Z (nm) | -0.22 | 0.139 | 0.225 |
| LDL.Z (nm) | 0.14 | 0.346 | 0.450 |
| HDL.Z (nm) | 0.34 | 0.024 | 0.077 |
| Non.HDL.P.(nmol/L) | 0.26 | 0.087 | 0.162 |
| Total.P.HDL.P (nmol/L) | 0.39 | 0.008 | 0.046 |
| LDL.P.HDL.P (nmol/L) | 0.39 | 0.008 | 0.046 |

**Rho: spearman’s correlation coefficient measures the strength of association between two variables; FDR: false discovery rate**

**Table S9:** Correlation of metabolites with survival time.

|  |  |  |
| --- | --- | --- |
| **Features** | **p-val** | **FDR** |
| Formate | 0.657 | 0.964 |
| Unknown signal at 8.12 ppm | 0.169 | 0.792 |
| Unknown signal at 8.07 ppm | 0.237 | 0.810 |
| Phenylalanine | 0.615 | 0.964 |
| Tyrosine | 0.895 | 0.964 |
| Unknown signal at 7.14 ppm | 0.865 | 0.964 |
| Histidine | 0.707 | 0.964 |
| Glucose | 0.919 | 0.964 |
| Mannose | 0.186 | 0.792 |
| Unknown signal at 5.15 ppm | 0.549 | 0.964 |
| Unknown signal at 5.09 ppm | 0.900 | 0.964 |
| Unknown signal at 5.01 ppm | 0.312 | 0.842 |
| Ascorbate | 0.379 | 0.919 |
| Threonine | 0.347 | 0.886 |
| Lactate | 0.852 | 0.964 |
| Creatinine | 0.929 | 0.964 |
| Creatine | 0.692 | 0.964 |
| Glycine | 0.236 | 0.810 |
| Methanol | 0.431 | 0.964 |
| Unknown signal at 2.55 ppm | 0.527 | 0.964 |
| Citrate | 0.083 | 0.760 |
| Glutamine | 0.500 | 0.964 |
| Pyruvate | 0.826 | 0.964 |
| Glutamate | 0.591 | 0.964 |
| Acetoacetate | 0.089 | 0.760 |
| Acetate | 0.837 | 0.964 |
| Alanine | 0.945 | 0.964 |
| Unknown signal at 1.45 ppm | 0.036 | 0.606 |
| Unknown signal at 1.43 ppm | 0.160 | 0.792 |
| 3-Hydroxybutyrate | 0.015 | 0.370 |
| Ethanol | 0.002 | 0.126 |
| Unknown signal at 1.16 ppm | 0.152 | 0.792 |
| Unknown signal at 1.14 ppm | 0.643 | 0.964 |
| Unknown signal at 1.11 ppm | 0.974 | 0.974 |
| Unknown signal at 1.06 ppm | 0.634 | 0.964 |
| Valine | 0.811 | 0.964 |
| Isoleucine | 0.512 | 0.964 |
| Leucine | 0.699 | 0.964 |
| 2-Hydroxybutyrate | 0.181 | 0.792 |
| Protein NH | 0.791 | 0.964 |
| Unsaturated lipid -CH=CH- | 0.451 | 0.964 |
| Lipid alpha-CH2 | 0.908 | 0.964 |
| Cholesterol | 0.059 | 0.752 |
| Lipid =CH-CH2-CH= | 0.270 | 0.810 |
| Glycorol phospholipid | 0.570 | 0.964 |
| Phospholipid | 0.159 | 0.792 |
| Lipid beta-CH2 | 0.560 | 0.964 |
| Lipid CH2 | 0.763 | 0.964 |
| Lipid CH3 | 0.314 | 0.842 |
| GlycB | 0.269 | 0.810 |
| GlycA | 0.257 | 0.810 |

**FDR: false discovery rate**

**Table S10:** Correlation of the lipid extracts with survival time

|  |  |  |
| --- | --- | --- |
| **Feature** | **p-val** | **FDR** |
| cholesterol-derivated 1 | 0.646 | 0.948 |
| cholesterol-derivated 2 | 0.664 | 0.948 |
| cholesterol-derivated 3 | 0.745 | 0.948 |
| cholesterol-derivated 4 | 0.783 | 0.948 |
| cholesterol-derivated 5 | 0.854 | 0.948 |
| free cholesterol | 0.722 | 0.948 |
| esterified cholesterol | 0.425 | 0.948 |
| cholesterol-derivated 6 | 0.245 | 0.948 |
| cholesterol-derivated 7 | 0.583 | 0.948 |
| cholesterol-derivated 8 | 0.785 | 0.948 |
| cholesterol-derivated 9 | 0.575 | 0.948 |
| saturated and omega-9 fatty acid | 0.710 | 0.948 |
| omega-7 fatty acid | 0.995 | 0.995 |
| omega-6 fatty acid | 0.486 | 0.948 |
| Unknown signal at | 0.508 | 0.948 |
| omega-3 fatty acid | 0.699 | 0.948 |
| monounsaturate fatty acid | 0.882 | 0.948 |
| polyunsaturate fatty acid 1 (except linoleic) | 0.588 | 0.948 |
| polyunsaturate fatty acid 2 (except linoleic) | 0.619 | 0.948 |
| linoleic acid | 0.908 | 0.948 |
| phosphatidylcholine | 0.697 | 0.948 |
| sphingomyelin | 0.603 | 0.948 |
| triglyceride | 0.682 | 0.948 |
| glycerophospholipid | 0.817 | 0.948 |

**FDR: false discovery rate**

**Table S11:** Correlation of metabolites ratios with survival time

|  |  |  |
| --- | --- | --- |
| **Features** | **p-val** | **FDR** |
| Glucose/Lactate | 0.741 | 0.873 |
| Pyruvate/Lactate | 0.873 | 0.873 |
| Threonine/Glycine | 0.721 | 0.873 |
| Glutamine/Glutamate | 0.473 | 0.788 |
| 3-Hydroxybutyrate/Acetoacetate | 0.241 | 0.783 |
| Glutamate/Alanine | 0.313 | 0.783 |

**FDR: false discovery rate**

**Table S12:** Correlation of lipoproteins with survival time

|  |  |  |
| --- | --- | --- |
| **Features** | **p-val** | **FDR** |
| VLDL.C (nmol/L) | 0.705 | 0.971 |
| IDL.C (nmol/L) | 0.699 | 0.971 |
| LDL.C (nmol/L) | 0.174 | 0.971 |
| HDL.C (nmol/L) | 0.666 | 0.971 |
| VLDL.TG (nmol/L) | 0.824 | 0.971 |
| IDL.TG (nmol/L) | 0.718 | 0.971 |
| LDL.TG (nmol/L) | 0.623 | 0.971 |
| HDL.TG (nmol/L) | 0.467 | 0.971 |
| VLDL.P (nmol/L) | 0.996 | 0.996 |
| Large.VLDL.P (nmol/L) | 0.771 | 0.971 |
| Medium.VLDL.P (nmol/L) | 0.581 | 0.971 |
| Small.VLDL.P.(nmol/L) | 0.935 | 0.973 |
| LDL.P (nmol/L) | 0.250 | 0.971 |
| Large.LDL.P (nmol/L) | 0.324 | 0.971 |
| Medium.LDL.P (nmol/L) | 0.379 | 0.971 |
| Small.LDL.P (nmol/L) | 0.136 | 0.971 |
| HDL.P (nmol/L) | 0.815 | 0.971 |
| Large.HDL.P (nmol/L) | 0.738 | 0.971 |
| Medium.HDL.P (nmol/L) | 0.884 | 0.971 |
| Small.HDL.P (nmol/L) | 0.627 | 0.971 |
| VLDL.Z (nm) | 0.776 | 0.971 |
| LDL.Z (nm) | 0.871 | 0.971 |
| HDL.Z (nm) | 0.404 | 0.971 |
| Non.HDL.P (nmol/L) | 0.271 | 0.971 |
| Total.P.HDL.P | 0.866 | 0.971 |
| LDL.P.HDL.P | 0.896 | 0.971 |

**FDR: false discovery rate**

**Table S13:** Comparison of the Full Blood Count of N versus AB Clusters

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Features** | **N, median [IQR]** | **AB, median [IQR]** | **logchange** | **p-val** | **FDR** |
| Haematocrit | 0.354 [0.312 0.392] | 0.28 [0.261 0.306] | -0.32 | 0.003 | 0.015 |
| white.cell.count (/L^9) | 7.315 [5.772 10.12] | 10.8 [8.27 15.04] | 0.73 | 0.011 | 0.040 |
| Haemaglobin (g/DL) | 11.2 [10.2 12.95] | 9.15 [8.725 9.85] | -0.29 | 0.002 | 0.015 |
| Platelet.count (/L^9) | 352.5 [250.75 450.5] | 410 [351.5 460.75] | 0.25 | 0.137 | 0.250 |
| Prothrombin.time (Sec) | 13.3 [12.4 14.8] | 14.2 [12.8 14.475] | 0.05 | 0.719 | 0.798 |
| INR | 1.08 [0.99 1.19] | 1.115 [1.032 1.168] | 0.06 | 0.639 | 0.798 |
| MCV (fL) | 92.3 [87.8 96.5] | 89.35 [87.625 95.65] | 0 | 0.826 | 0.826 |
| MCH (pg) | 30.2 [28.1 31.4] | 29.8 [28.825 32.1] | 0.03 | 0.725 | 0.798 |
| MCHC (g/dl) | 32.7 [31.3 33.4] | 33.5 [32.2 34.15] | 0.03 | 0.131 | 0.250 |
| MPV (fL) | 10.5 [9.475 10.8] | 10.75 [9.825 11.2] | 0.05 | 0.172 | 0.271 |
| Red.cell.count.(/L^12) | 3.77 [3.42 4.54] | 2.985 [2.75 3.473] | -0.12 | 0.020 | 0.055 |

**IQR: Interquartile range; FDR: false discovery rate**

**Table S14:** Comparison of the Blood chemistry of N versus AB components

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Feature** | **N, median [IQR]** | **AB, median [IQR]** | **logchange** | **p-val** | **FDR** |
| Sodium (mmol/L) | 138 [135 140] | 136.5 [130.5 138.5] | -0.04 | 0.063 | 0.260 |
| Potassium (mmol/L) | 3.8 [3.4 4.5] | 3.65 [3.35 3.875] | -0.08 | 0.403 | 0.448 |
| Chloride (mmol/L) | 97 [93 99] | 93 [91.25 96] | -0.04 | 0.078 | 0.260 |
| Bicarbonate (mmol.L. | 21 [19 24] | 18.5 [17 24] | -0.14 | 0.186 | 0.321 |
| Anion.gap. (mmol/L) | 23 [20 27] | 27.5 [21.25 30.75] | 0.07 | 0.395 | 0.448 |
| Calcium(mmol/L) | 2.2 [2.13 2.32] | 2.14 [1.997 2.223] | -0.14 | 0.107 | 0.267 |
| Magnesium (mmol/L) | 0.84 [0.79 0.92] | 0.72 [0.673 0.753] | -0.29 | 0.019 | 0.190 |
| Inorganic.Phosphate (mmol/L) | 1.13 [1.03 1.26] | 1.02 [0.938 1.198] | -0.16 | 0.192 | 0.321 |
| Urea (mmol/L) | 4.3 [2.9 5.6] | 3.25 [2 8.175] | 0.17 | 0.747 | 0.747 |
| Creatinine (µmol/L) | 75 [63 97] | 62.5 [52.75 88.75] | -0.22 | 0.266 | 0.380 |

**IQR: Interquartile range; FDR: false discovery rate**

**Table S15:** Comparison of the Liver function tests of N versus AB components

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Feature** | **N, median [IQR]** | **AB, median [IQR]** | **logchange** | **p-val** | **FDR** |
| Total.Protein.(g/L) | 68 [59 76] | 58 [53 64] | -0.23 | 0.018 | 0.029 |
| Albumin.(g/L) | 36 [28 40] | 27.5 [26.25 29.75] | -0.34 | 0.002 | 0.012 |
| Total.Bilirubin (µmol/L) | 43 [8 100] | 174.5 [143.25 266] | 1.32 | 0.003 | 0.012 |
| Conjugated.Bilirubin (µmol/L) | 31 [3 97] | 146 [126.75 241.5] | 1.34 | 0.006 | 0.016 |
| Alanine.transaminase (U/L) | 28 [18 71] | 81.5 [23.25 113.25] | 0.2 | 0.371 | 0.425 |
| Aspartate.transaminase (U/L) | 42 [24 92] | 115.5 [83 148.5] | 0.82 | 0.009 | 0.018 |
| Alkaline.phosphatase (U/L) | 288 [103 683] | 696 [330.25 1378.25] | 0.62 | 0.044 | 0.059 |
| Gamma.glutamyl.transferase (U/L) | 307 [77 1021] | 394 [208 926.25] | -0.04 | 0.650 | 0.650 |

**IQR: Interquartile range; FDR: false discovery rate**

**Table S16:** Comparison of the metabolite concentration of N versus AB clusters

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Features** | **N (mM), median [IQR]** | **AB (mM), median [IQR]** | **logchange** | **p-val** | **FDR** |
| Formate | 0.016 [0.011 0.019] | 0.019 [0.016 0.022] | 0.24 | 0.067 | 0.225 |
| Unknown signal at 8.12 ppm | 0 [0 0.007] | 0 [0 0.023] | 1.18 | 0.304 | 0.550 |
| Unknown signal at 8.07 ppm | 0 [0 0.005] | 0 [0 0.01] | 1 | 0.193 | 0.411 |
| Phenylalanine | 0.104 [0.069 0.128] | 0.113 [0.102 0.143] | 0.14 | 0.080 | 0.225 |
| Tyrosine | 0.046 [0.036 0.052] | 0.04 [0.035 0.054] | -0.44 | 0.585 | 0.787 |
| Unknown signal at 7.14 ppm | 0.026 [0 0.079] | 0.034 [0 0.052] | -0.78 | 0.820 | 0.889 |
| Histidine | 0.064 [0.055 0.082] | 0.074 [0.064 0.078] | -0.01 | 0.313 | 0.550 |
| Glucose | 3.532 [3.029 4.205] | 3.549 [2.546 4.962] | 0.13 | 0.952 | 0.980 |
| Mannose | 0.037 [0.028 0.051] | 0.078 [0.037 0.115] | 1.06 | 0.005 | 0.029 |
| Unknown signal at 5.15 ppm | 0 [0 0] | 0 [0 0] | 0.23 | 0.607 | 0.787 |
| Unknown signal at 5.09 ppm | 0 [0 0.043] | 0 [0 0.032] | -0.67 | 0.696 | 0.845 |
| Unknown signal at 5.01 ppm | 0 [0 0] | 0 [0 0] | 0.99 | 0.151 | 0.340 |
| Ascorbate | 0.01 [0 0.019] | 0 [0 0.014] | -0.6 | 0.397 | 0.621 |
| Threonine | 0.079 [0.06 0.091] | 0 [0 0.043] | -1.47 | 0.002 | 0.013 |
| Lactate | 2.253 [2.013 3.114] | 2.927 [2.62 3.179] | -0.01 | 0.153 | 0.340 |
| Creatinine | 0.057 [0.044 0.073] | 0.053 [0.031 0.076] | -0.11 | 0.520 | 0.781 |
| Creatine | 0.012 [0.006 0.035] | 0.002 [0 0.028] | -0.56 | 0.089 | 0.227 |
| Glycine | 0.318 [0.242 0.354] | 0.311 [0.273 0.353] | -0.12 | 0.952 | 0.980 |
| Methanol | 0.027 [0.018 0.036] | 0.021 [0.013 0.023] | -0.55 | 0.054 | 0.219 |
| Unknown signal at 2.55 ppm | 0 [0 0.013] | 0 [0 0.013] | -3.27 | 0.589 | 0.787 |
| Citrate | 0.081 [0 0.103] | 0.09 [0 0.123] | -0.11 | 0.100 | 0.100 |
| Glutamine | 0.4 [0.294 0.424] | 0.268 [0.197 0.294] | -0.57 | <0.001 | 0.007 |
| Pyruvate | 0.058 [0.048 0.072] | 0.061 [0.047 0.091] | 0.08 | 0.762 | 0.883 |
| Glutamate | 0.19 [0.129 0.272] | 0.202 [0.155 0.285] | 0.09 | 0.402 | 0.621 |
| Acetoacetate | 0.019 [0.016 0.041] | 0.025 [0.017 0.089] | 0.09 | 0.301 | 0.550 |
| Acetate | 0.024 [0.02 0.033] | 0.032 [0.026 0.039] | 0.09 | 0.120 | 0.292 |
| Alanine | 0.395 [0.293 0.481] | 0.341 [0.273 0.35] | -0.56 | 0.051 | 0.219 |
| Unknown signal at 1.45 ppm | 0.031 [0.024 0.039] | 0.02 [0 0.049] | -0.18 | 0961 | 0.980 |
| Unknown signal at 1.43 ppm | 0 [0 0] | 0 [0 0.405] | 1.85 | 0.005 | 0.029 |
| 3-Hydroxybutyrate | 0.046 [0.028 0.1] | 0.05 [0.037 0.451] | 0.73 | 0.580 | 0.787 |
| Ethanol | 0.022 [0 0.083] | 0 [0 0.084] | -0.81 | 0.389 | 0.621 |
| Unknown signal at 1.16 ppm | 0.112 [0 0.297] | 0.168 [0.026 0.337] | 0.08 | 0.610 | 0.787 |
| Unknown signal at 1.14 ppm | 0.019 [0 0.043] | 0.016 [0 0.029] | -0.81 | 0.729 | 0.865 |
| Unknown signal at 1.11 ppm | 0.053 [0.044 0.061] | 0.061 [0.041 0.073] | 0.01 | 0.633 | 0.787 |
| Unknown signal at 1.06 ppm | 0.029 [0.021 0.038] | 0.044 [0.026 0.067] | 0.24 | 0.057 | 0.219 |
| Valine | 0.163 [0.127 0.183] | 0.139 [0.105 0.161] | -0.35 | 0.084 | 0.225 |
| Isoleucine | 0.041 [0.033 0.053] | 0.046 [0.042 0.054] | 0.06 | 0.391 | 0.621 |
| Leucine | 0.068 [0.055 0.075] | 0.05 [0.042 0.067] | -0.59 | 0.021 | 0.108 |
| 2-Hydroxybutyrate | 0 [0 0.021] | 0.009 [0 0.048] | 1.07 | 0.312 | 0.550 |
| Protein NH | 144.358 [121.287 154.93] | 105.798 [104.188 112.176] | -0.36 | <0.001 | <0.001 |
| Unsaturated lipid -CH=CH- | 11.141 [8.332 14.097] | 14.379 [9.344 19.988] | 0.36 | 0.080 | 0.225 |
| Lipid alpha-CH2 | 1.863 [1.252 2.379] | 6.257 [4.119 8.056] | 1.7 | <0.001 | <0.001 |
| Cholesterol | 0.825 [0.644 1.064] | 0.516 [0.27 0.934] | -0.37 | 0.060 | 0.219 |
| Lipid =CH-CH2-CH= | 4.954 [3.999 6.138] | 5.02 [3.569 7.556] | 0.17 | 0.818 | 0.889 |
| Glycorol phospholipid | 0.487 [0.243 0.77] | 1.663 [1.412 2.797] | 1.94 | <0.001 | <0.001 |
| Phospholipid | 3.699 [3.478 4.142] | 3.128 [2.95 3.39] | -0.24 | <0.001 | 0.005 |
| Lipid beta-CH2 | 7.403 [5.083 8.55] | 10.095 [6.281 12.356] | 0.35 | 0.084 | 0.225 |
| Lipid CH2 | 62.251 [55.441 75.596] | 111.18 [73.472 140.862] | 0.71 | <0.001 | 0.001 |
| Lipid CH3 | 26.385 [21.436 29.909] | 27.943 [23.387 34.927] | 0.14 | 0.279 | 0.550 |
| GlycB | 0.406 [0.322 0.471] | 0.407 [0.366 0.436] | -0.04 | 0.799 | 0.889 |
| GlycA | 1.996 [1.535 2.186] | 1.833 [1.701 2.005] | -0.03 | 0.619 | 0.787 |

**IQR: Interquartile range; FDR: false discovery rate**

**Table S17:** Comparison of the lipid extracts concentration of N versus AB clusters.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Feature** | **N, median [IQR]** | **AB, median [IQR]** | **logchange** | **p-val** | **FDR** |
| cholesterol-derivated 1 | 0.661 [0.571 0.791] | 1.46 [1.158 1.675] | 0.88 | <0.001 | <0.001 |
| cholesterol-derivated 2 | 0.613 [0.537 0.75] | 1.484 [1.15 1.745] | 0.97 | <0.001 | <0.001 |
| cholesterol-derivated 3 | 0.805 [0.694 0.893] | 1.273 [1.118 1.327] | 0.48 | <0.001 | <0.001 |
| cholesterol-derivated 4 | 0.639 [0.569 0.778] | 1.424 [1.185 1.641] | 0.85 | <0.001 | <0.001 |
| cholesterol-derivated 5 | 1.299 [0.909 1.667] | 0.271 [0.241 0.385] | -2.14 | <0.001 | <0.001 |
| free cholesterol | 0.193 [0.055 0.271] | 2.095 [0.96 3.516] | 2.52 | <0.001 | <0.001 |
| esterified cholesterol | 0.93 [0.572 1.271] | 1.073 [0.343 1.437] | -0.03 | 0.977 | 0.977 |
| cholesterol-derivated 6 | 0.608 [0.526 0.828] | 1.54 [0.835 2.05] | 0.99 | 0.002 | 0.002 |
| cholesterol-derivated 7 | 1.069 [0.907 1.394] | 0.713 [0.604 0.784] | -0.67 | <0.001 | <0.001 |
| cholesterol-derivated 8 | 0.607 [0.547 0.822] | 1.468 [1.162 1.69] | 0.9 | <0.001 | <0.001 |
| cholesterol-derivated 9 | 1.127 [0.747 1.75] | 0.333 [0.31 0.401] | -1.87 | <0.001 | <0.001 |
| saturated and omega-9 fatty acid | 0.667 [0.538 0.833] | 1.443 [1.223 1.999] | 1.07 | <0.001 | <0.001 |
| omega-7 fatty acid | 0.909 [0.78 1.043] | 1.126 [0.982 1.221] | 0.36 | 0.002 | 0.002 |
| omega-6 fatty acid | 0.583 [0.367 1.078] | 1.448 [1.256 1.851] | 1.07 | <0.001 | <0.001 |
| Unknown signal at 0.91 ppm | 0 [0 0] | 0 [0 0] |  | 0.230 | 0.240 |
| omega-3 fatty acid | 0.626 [0.397 0.798] | 1.748 [1.159 1.915] | 1.14 | <0.001 | <0.001 |
| monounsaturate fatty acid | 0.38 [0.193 0.656] | 1.898 [1.386 2.441] | 2.06 | <0.001 | <0.001 |
| polyunsaturate fatty acid 1 | 0.552 [0.342 0.832] | 1.63 [1.211 2.031] | 1.46 | <0.001 | <0.001 |
| polyunsaturate fatty acid 2 | 0.536 [0.334 0.812] | 1.736 [1.327 2.057] | 1.47 | <0.001 | <0.001 |
| linoleic acid | 0.476 [0.228 0.756] | 1.582 [1.234 2.454] | 1.53 | <0.001 | <0.001 |
| phosphatidylcholine | 0.533 [0.419 0.669] | 1.624 [1.108 2.288] | 1.52 | <0.001 | <0.001 |
| sphingomyelin | 0.594 [0.499 0.833] | 1.205 [0.928 1.719] | 0.97 | <0.001 | <0.001 |
| triglyceride | 0.59 [0.474 0.838] | 1.643 [1.413 2.011] | 1.41 | <0.001 | <0.001 |
| glycerophospholipid | 0.494 [0.393 0.614] | 1.704 [1.26 2.384] | 1.65 | <0.001 | <0.001 |

**IQR: Interquartile range; FDR: false discovery rate**

**Table S18:** Comparison of the metabolites ratio concentration of N versus AB clusters.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Feature** | **N, median [IQR]** | **AB, median [IQR]** | **logchange** | **p-val** | **FDR** |
| Glucose/Pyruvate | 1.483 [1.254 1.769] | 1.201 [0.975 1.774] | 0.1 | 0.459 | 0.689 |
| Pyruvate/Lactate | 0.023 [0.019 0.031] | 0.027 [0.017 0.029] | -0.05 | 0.799 | 0.912 |
| Threonine/Glycine | 0.248 [0.207 0.31] | 0 [0 0.152] | -1.51 | 0.004 | 0.019 |
| Glutamine/Glutamate | 1.966 [1.23 3.538] | 1.378 [0.704 2.113] | -0.8 | 0.029 | 0.048 |
| 3-Hydroxybutyrate/Acetoacetate | 2.566 [1.258 3.729] | 2.415 [0.865 4.247] | 0.11 | 0.912 | 0.912 |
| Glutamate/Alanine | 0.52 [0.358 0.606] | 0.634 [0.516 0.976] | 0.59 | 0.013 | 0.031 |

**IQR: Interquartile range; FDR: false discovery rate**

**Table S19:** Comparison of the lipoprotein profile for N versus AB clusters

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Feature** | **N, median [IQR]** | **AB, median [IQR]** | **logchange** | **p-val** | **FDR** |
| VLDL.C (nmol/L) | 17.81 [11.205 24.26] | 24.08 [16.92 34.872] | 0.58 | 0.025 | 0.030 |
| IDL.C (nmol/L) | 17.31 [10.345 21.475] | 73.96 [52.33 82.738] | 1.91 | <0.001 | <0.001 |
| LDL.C (nmol/L) | 108.36 [87.245 130.24] | 146.94 [119.998 165.042] | 0.38 | 0.008 | 0.010 |
| HDL.C (nmol/L) | 36.31 [28.005 50.43] | 1 [1 1] | -4.99 | <0.001 | <0.001 |
| VLDL.TG (nmol/L) | 73.84 [47.195 92.89] | 108.86 [82.815 141.52] | 0.77 | <0.001 | 0.001 |
| IDL.TG (nmol/L) | 15.4 [11.215 18.165] | 50.75 [35.712 57.97] | 1.55 | <0.001 | <0.001 |
| LDL.TG (nmol/L) | 18.96 [11.86 30.375] | 72.13 [48.785 85.205] | 1.59 | <0.001 | <0.001 |
| HDL.TG (nmol/L) | 17.76 [15.12 22.85] | 24.345 [13.485 30.7] | 0.25 | 0.459 | 0.459 |
| VLDL.P (nmol/L) | 50.87 [33.49 65.585] | 79.76 [56.802 104.332] | 0.75 | <0.001 | 0.001 |
| Large.VLDL.P.(nmol/L) | 1.38 [0.875 1.61] | 1.445 [1.375 1.7] | 0.39 | 0.095 | 0.103 |
| Medium.VLDL.P (nmol./L) | 5.53 [4.03 7.4] | 5.465 [5.07 7.022] | 0.31 | 0.440 | 0.458 |
| Small.VLDL.P..(nmol/L) | 43.15 [29.4 56.13] | 74.645 [50.73 96.23] | 0.8 | <0.001 | <0.001 |
| LDL.P (nmol/L) | 1113.73 [848.825 1331.92] | 1745.03 [1458.052 2184.075] | 0.66 | <0.001 | <0.001 |
| Large.LDL.P.(nmol/L) | 180.92 [131.475 215.42] | 268.655 [194.603 301.295] | 0.45 | 0.002 | <0.001 |
| Medium.LDL.P.(nmol/L) | 349.05 [194.215 521.08] | 868.56 [666.858 1136.122] | 1.12 | <0.001 | <0.001 |
| Small.LDL.P (nmol/L) | 577.17 [480.125 661.975] | 634.715 [559.785 805.162] | 0.29 | 0.084 | 0.095 |
| HDL.P (mol/L) | 18.54 [14.905 25.96] | 4.855 [2.812 5.335] | -2.13 | <0.001 | <0.001 |
| Large.HDL.P (mol/L) | 0.28 [0.245 0.305] | 0.175 [0.105 0.223] | -0.78 | <0.001 | <0.001 |
| Medium.HDL.P.(mol/L) | 10.55 [9.295 11.395] | 5.735 [3.708 6.16] | -1 | <0.001 | <0.001 |
| Small.HDL.P.(mol/L) | 8.87 [3.175 15.98] | 0 [0 0] | -5.7 | <0.001 | <0.001 |
| VLDL.Z (nm) | 42.2 [42.175 42.22] | 42.16 [42.13 42.18] | 0 | 0.001 | 0.002 |
| LDL.Z (nm) | 21.27 [21.135 21.46] | 21.595 [21.505 21.655] | 0.02 | <0.001 | <0.001 |
| HDL.Z (nm) | 8.5 [8.34 8.9] | 9.55 [9.47 9.645] | 0.15 | <0.001 | <0.001 |
| Non.HDL.P.(nmol/L) | 1130.02 [847.865 1358.64] | 1838.72 [1510.072 2274.648] | 0.68 | <0.001 | <0.001 |
| Total.P.HDL.P (nmol/L) | 48.14 [35.675 98.015] | 437.875 [354.01 539.432] | 2.64 | <0.001 | <0.001 |
| LDL.P.HDL.P (nmol/L) | 43.99 [34.045 95.405] | 414.975 [333.365 517.24] | 2.63 | <0.001 | <0.001 |

**IQR: Interquartile range; FDR: false discovery rate**

**Table S20:** Correlation of metabolites with GlycA, GlycB, CRP, and Albumin intensity value.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **GlycA** | | |  | **GlycB** | | |  | **CRP** | | |  | **Albumin** | | |
| **Feature** | **rho** | **p-value** | **FDR** |  | **rho** | **p-value** | **FDR** |  | **rho** | **p-value** | **FDR** |  | **rho** | **p-value** | **FDR** | |
| Formate | 0.2 | 0.186 | 0.389 |  | 0.27 | 0.072 | 0.334 |  | 0.08 | 0.656 | 0.910 |  | -0.27 | 0.101 | 0.477 | |
| Unknown signal at 8.12 ppm | -0.27 | 0.068 | 0.233 |  | -0.23 | 0.122 | 0.367 |  | -0.08 | 0.636 | 0.910 |  | -0.14 | 0.387 | 0.658 | |
| Unknown signal at 8.07 ppm | -0.26 | 0.079 | 0.233 |  | -0.16 | 0.304 | 0.583 |  | 0.03 | 0.847 | 0.910 |  | -0.19 | 0.237 | 0.526 | |
| Phenylalanine | 0.2 | 0.190 | 0.389 |  | 0.29 | 0.055 | 0.280 |  | 0.29 | 0.079 | 0.808 |  | -0.21 | 0.197 | 0.523 | |
| Tyrosine | -0.33 | 0.027 | 0.175 |  | -0.26 | 0.079 | 0.335 |  | 0.06 | 0.727 | 0.910 |  | 0.06 | 0.702 | 0.904 | |
| Unknown signal at 7.14 ppm | 0.34 | 0.021 | 0.157 |  | 0.26 | 0.090 | 0.346 |  | 0.08 | 0.622 | 0.910 |  | -0.26 | 0.115 | 0.477 | |
| Histidine | -0.56 | <0.001 | 0.001 |  | -0.49 | <0.001 | 0.008 |  | -0.16 | 0.358 | 0.829 |  | 0.07 | 0.662 | 0.904 | |
| Glucose | 0.27 | 0.727 | 0.233 |  | 0.36 | 0.015 | 0.095 |  | -0.22 | 0.184 | 0.829 |  | 0.05 | 0.740 | 0.904 | |
| Mannose | 0.34 | 0.021 | 0.157 |  | 0.36 | 0.115 | 0.095 |  | 0.04 | 0.832 | 0.910 |  | -0.21 | 0.192 | 0.523 | |
| Unknown signal at 5.15 ppm | -0.25 | 0.096 | 0.233 |  | -0.14 | 0.358 | 0.593 |  | -0.06 | 0.738 | 0.910 |  | -0.18 | 0.269 | 0.553 | |
| Unknown signal at 5.09 ppm | 0.26 | 0.086 | 0.233 |  | 0.18 | 0.233 | 0.583 |  | -0.01 | 0.950 | 0.969 |  | -0.29 | 0.076 | 0.477 | |
| Unknown signal at 5.01 ppm | -0.28 | 0.061 | 0.233 |  | -0.16 | 0.286 | 0.583 |  | 0.07 | 0.692 | 0.910 |  | -0.24 | 0.140 | 0.477 | |
| Ascorbate | -0.25 | 0.095 | 0.233 |  | -0.25 | 0.099 | 0.346 |  | -0.05 | 0.749 | 0.910 |  | -0.04 | 0.806 | 0.909 | |
| Threonine | 0.04 | 0.807 | 0.895 |  | 0.02 | 0.878 | 0.904 |  | -0.16 | 0.344 | 0.829 |  | 0.3 | 0.064 | 0.477 | |
| Lactate | 0.32 | 0.031 | 0.176 |  | 0.38 | 0.009 | 0.082 |  | 0.4 | 0.014 | 0.559 |  | -0.2 | 0.218 | 0.523 | |
| Creatinine | -0.1 | 0.506 | 0.842 |  | -0.06 | 0.693 | 0.803 |  | -0.06 | 0.711 | 0.910 |  | -0.04 | 0.820 | 0.909 | |
| Creatine | -0.06 | 0.675 | 0.842 |  | -0.03 | 0.862 | 0.904 |  | 0.2 | 0.228 | 0.829 |  | 0 | 0.993 | 0.993 | |
| Glycine | 0.07 | 0.643 | 0.842 |  | 0.13 | 0.397 | 0.610 |  | 0.16 | 0.356 | 0.829 |  | -0.22 | 0.180 | 0.523 | |
| Methanol | -0.03 | 0.848 | 0.920 |  | -0.18 | 0.237 | 0.583 |  | 0.04 | 0.830 | 0.910 |  | 0.35 | 0.028 | 0.283 | |
| Unknown signal at 2.55 ppm | 0.08 | 0.619 | 0.842 |  | -0.05 | 0.768 | 0.851 |  | -0.16 | 0.341 | 0.829 |  | 0.22 | 0.169 | 0.523 | |
| Citrate | -0.18 | 0.237 | 0.465 |  | -0.06 | 0.710 | 0.805 |  | -0.08 | 0.642 | 0.910 |  | -0.09 | 0.599 | 0.872 | |
| Glutamine | -0.06 | 0.694 | 0.842 |  | -0.16 | 0.300 | 0.583 |  | -0.25 | 0.137 | 0.829 |  | 0.05 | 0.773 | 0.909 | |
| Pyruvate | 0.15 | 0.340 | 0.598 |  | 0.24 | 0.109 | 0.346 |  | 0.19 | 0.270 | 0.829 |  | -0.24 | 0.135 | 0.477 | |
| Glutamate | 0.02 | 0.879 | 0.934 |  | 0.07 | 0.645 | 0.783 |  | 0.09 | 0.595 | 0.910 |  | -0.06 | 0.733 | 0.904 | |
| Acetoacetate | -0.3 | 0.049 | 0.233 |  | -0.16 | 0.283 | 0.583 |  | -0.03 | 0.857 | 0.910 |  | -0.12 | 0.455 | 0.737 | |
| Acetate | -0.17 | 0.277 | 0.523 |  | -0.08 | 0.596 | 0.760 |  | -0.03 | 0.857 | 0.910 |  | -0.16 | 0.318 | 0.588 | |
| Alanine | -0.1 | 0.531 | 0.842 |  | -0.12 | 0.413 | 0.610 |  | -0.07 | 0.695 | 0.910 |  | 0.25 | 0.124 | 0.477 | |
| Unknown signal at 1.45 ppm | 0.6 | <0.001 | <0.001 |  | 0.65 | <0.001 | <0.001 |  | 0.36 | 0.028 | 0.559 |  | -0.07 | 0.657 | 0.904 | |
| Unknown signal at 1.43 ppm | -0.29 | 0.055 | 0.233 |  | -0.24 | 0.108 | 0.346 |  | 0.04 | 0.814 | 0.910 |  | -0.28 | 0.087 | 0.477 | |
| 3-Hydroxybutyrate | -0.06 | 0.677 | 0.842 |  | 0 | 0.977 | 0.977 |  | 0.12 | 0.475 | 0.910 |  | -0.06 | 0.708 | 0.904 | |
| Ethanol | -0.05 | 0.726 | 0.842 |  | -0.06 | 0.673 | 0.798 |  | 0 | 0.998 | 0.998 |  | -0.11 | 0.493 | 0.761 | |
| Unknown signal at 1.16 ppm | 0.06 | 0.713 | 0.842 |  | 0.12 | 0.430 | 0.610 |  | -0.16 | 0.347 | 0.829 |  | -0.16 | 0.320 | 0.588 | |
| Unknown signal at 1.14 ppm | 0.22 | 0.149 | 0.330 |  | 0.15 | 0.338 | 0.593 |  | 0.17 | 0.321 | 0.829 |  | 0.12 | 0.462 | 0.737 | |
| Unknown signal at 1.11 ppm | 0 | 0.999 | 0.999 |  | 0.11 | 0.490 | 0.657 |  | -0.07 | 0.697 | 0.910 |  | 0 | 0.993 | 0.993 | |
| Unknown signal at 1.06 ppm | -0.26 | 0.090 | 0.233 |  | -0.17 | 0.257 | 0.583 |  | 0.12 | 0.480 | 0.910 |  | -0.16 | 0.323 | 0.588 | |
| Valine | -0.08 | 0.611 | 0.842 |  | -0.12 | 0.443 | 0.611 |  | -0.07 | 0.682 | 0.910 |  | 0.2 | 0.226 | 0.523 | |
| Isoleucine | 0.25 | 0.103 | 0.238 |  | 0.15 | 0.325 | 0.591 |  | -0.02 | 0.920 | 0.957 |  | -0.11 | 0.510 | 0.766 | |
| Leucine | 0.09 | 0.536 | 0.842 |  | 0.09 | 0.572 | 0.748 |  | 0.09 | 0.585 | 0.910 |  | 0.26 | 0.116 | 0.477 | |
| 2-Hydroxybutyrate | -0.28 | 0.065 | 0.233 |  | -0.14 | 0.361 | 0.593 |  | 0.12 | 0.465 | 0.910 |  | -0.03 | 0.880 | 0.954 | |
| Protein NH | 0.08 | 0.610 | 0.842 |  | -0.03 | 0.831 | 0.902 |  | -0.17 | 0.317 | 0.829 |  | 0.7 | <0.001 | <0.001 | |
| Unsaturated lipid -CH=CH- | -0.09 | 0.567 | 0.842 |  | -0.16 | 0.286 | 0.583 |  | 0.23 | 0.174 | 0.829 |  | 0.04 | 0.786 | 0.909 | |
| Lipid alpha-CH2 | -0.09 | 0.567 | 0.842 |  | -0.13 | 0.397 | 0.610 |  | 0.33 | 0.043 | 0.559 |  | -0.43 | 0.006 | 0.157 | |
| Cholesterol | 0.01 | 0.926 | 0.964 |  | -0.02 | 0.886 | 0.904 |  | -0.04 | 0.825 | 0.910 |  | 0.27 | 0.099 | 0.477 | |
| Lipid =CH-CH2-CH= | 0 | 0.986 | 0.999 |  | -0.08 | 0.621 | 0.773 |  | 0.2 | 0.230 | 0.829 |  | 0.18 | 0.271 | 0.553 | |
| Glycorol phospholipid | -0.16 | 0.306 | 0.557 |  | -0.21 | 0.172 | 0.488 |  | 0.25 | 0.143 | 0.829 |  | -0.37 | 0.019 | 0.243 | |
| Phospholipid | 0.42 | 0.004 | 0.041 |  | 0.41 | 0.005 | 0.055 |  | 0.06 | 0.703 | 0.910 |  | 0.4 | 0.012 | 0.198 | |
| Lipid beta-CH2 | -0.27 | 0.073 | 0.233 |  | -0.32 | 0.031 | 0.178 |  | 0.13 | 0.458 | 0.910 |  | -0.02 | 0.917 | 0.974 | |
| Lipid CH2 | -0.07 | 0.647 | 0.842 |  | -0.15 | 0.309 | 0.583 |  | 0.33 | 0.043 | 0.559 |  | -0.2 | 0.213 | 0.523 | |
| Lipid CH3 | -0.04 | 0.801 | 0.895 |  | -0.12 | 0.424 | 0.610 |  | 0.19 | 0.262 | 0.829 |  | 0.16 | 0.340 | 0.598 | |
| GlycB | 0.9 | 0.00E+00 | 0.00E+00 |  | 1 | 0.00E+00 | 0.00E+00 |  | 0.22 | 0.195 | 0.829 |  | 0.01 | 0.969 | 0.993 | |
| GlycA | 1 | 0.00E+00 | 0.00E+00 |  | 0.9 | 0.00E+00 | 0.00E+00 |  | 0.26 | 0.115 | 0.829 |  | 0.05 | 0.744 | 0.904 | |

**Rho: spearman’s correlation coefficient measures the strength of association between two variables; FDR: false discovery rate**

**Table S21:** Correlation of lipid extracts with GlycA, GlycB, CRP, and Albumin intensity value

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **GlycA** | | |  | **GlycB** | | | |  | | **CRP** | | | |  | | **Albumin** | | | |
| **Feature** | **rho** | **p-value** | **FDR** |  | **rho** | **p-value** | **FDR** |  | | **rho** | | **p-value** | **FDR** |  | | **rho** | | **p-value** | **FDR** |
| cholesterol-derivated 1 | -0.17 | 0.296 | 0.666 |  | -0.11 | 0.502 | 0.788 |  | | 0.35 | | 0.045 | 0.123 |  | | -0.54 | | <0.001 | 0.006 |
| cholesterol-derivated 2 | -0.16 | 0.328 | 0.666 |  | -0.1 | 0.525 | 0.788 |  | | 0.37 | | 0.035 | 0.123 |  | | -0.53 | | 0.001 | 0.006 |
| cholesterol-derivated 3 | -0.22 | 0.172 | 0.666 |  | -0.17 | 0.282 | 0.788 |  | | 0.41 | | 0.019 | 0.123 |  | | -0.5 | | 0.002 | 0.007 |
| cholesterol-derivated 4 | -0.17 | 0.299 | 0.666 |  | -0.12 | 0.458 | 0.788 |  | | 0.37 | | 0.035 | 0.123 |  | | -0.54 | | <0.001 | 0.006 |
| cholesterol-derivated 5 | 0.11 | 0.511 | 0.756 |  | 0.05 | 0.775 | 0.829 |  | | -0.35 | | 0.044 | 0.123 |  | | 0.51 | | 0.002 | 0.006 |
| free cholesterol | -0.18 | 0.273 | 0.666 |  | -0.13 | 0.440 | 0.788 |  | | 0.3 | | 0.094 | 0.174 |  | | -0.39 | | 0.020 | 0.044 |
| esterified cholesterol | -0.04 | 0.815 | 0.857 |  | -0.13 | 0.414 | 0.788 |  | | -0.09 | | 0.632 | 0.632 |  | | 0.34 | | 0.044 | 0.082 |
| cholesterol-derivated 6 | -0.14 | 0.397 | 0.666 |  | -0.04 | 0.798 | 0.829 |  | | 0.26 | | 0.146 | 2.00 |  | | -0.56 | | <0.001 | 0.060 |
| cholesterol-derivated 7 | -0.06 | 0.701 | 0.857 |  | -0.04 | 0.829 | 0.829 |  | | -0.35 | | 0.046 | 0.123 |  | | 0.27 | | 0.117 | 0.165 |
| cholesterol-derivated 8 | -0.16 | 0.338 | 0.666 |  | -0.11 | 0.490 | 0.788 |  | | 0.37 | | 0.035 | 0.123 |  | | -0.51 | | 0.002 | 0.006 |
| cholesterol-derivated 9 | 0.1 | 0.535 | 0.756 |  | 0.1 | 0.545 | 0.788 |  | | -0.39 | | 0.027 | 0.123 |  | | 0.51 | | 0.002 | 0.006 |
| saturated and omega-9 fatty acid | -0.23 | 0.156 | 0.666 |  | -0.14 | 0.372 | 0.788 |  | | 0.32 | | 0.071 | 0.172 |  | | -0.44 | | 0.009 | 0.022 |
| omega-7 fatty acid | -0.03 | 0.857 | 0.857 |  | -0.05 | 0.736 | 0.829 |  | | 0.18 | | 0.321 | 0.335 |  | | -0.47 | | 0.004 | 0.011 |
| omega-6 fatty acid | -0.07 | 0.648 | 0.857 |  | -0.1 | 0.558 | 0.788 |  | | 0.23 | | 0.196 | 0.235 |  | | -0.19 | | 0.285 | 0.285 |
| Unknown signal at 0.91 ppm | -0.03 | 0.837 | 0.857 |  | -0.11 | 0.488 | 0.788 |  | | 0.19 | | 0.288 | 0.314 |  | | -0.24 | | 0.163 | 0.218 |
| omega-3 fatty acid | -0.16 | 0.323 | 0.666 |  | -0.09 | 0.602 | 0.803 |  | | 0.2 | | 0.273 | 0.312 |  | | -0.29 | | 0.095 | 0.142 |
| monounsaturate fatty acid | -0.13 | 0.417 | 0.666 |  | -0.1 | 0.539 | 0.788 |  | | 0.3 | | 0.093 | 0.174 |  | | -0.36 | | 0.033 | 0.065 |
| polyunsaturate fatty acid 1 | -0.14 | 0.376 | 0.666 |  | -0.13 | 0.425 | 0.788 |  | | 0.28 | | 0.110 | 0.188 |  | | -0.19 | | 0.284 | 0.285 |
| polyunsaturate fatty acid 2 | -0.19 | 0.245 | 0.666 |  | -0.16 | 0.326 | 0.788 |  | | 0.26 | | 0.150 | 2.00 |  | | -0.21 | | 0.233 | 0.266 |
| linoleic acid | -0.17 | 0.282 | 0.666 |  | -0.14 | 0.390 | 0.788 |  | | 0.26 | | 0.147 | 2.00 |  | | -0.22 | | 0.200 | 0.240 |
| phosphatidylcholine | -0.19 | 0.237 | 0.666 |  | -0.16 | 0.316 | 0.788 |  | | 0.27 | | 0.130 | 2.00 |  | | -0.32 | | 0.063 | 0.100 |
| sphingomyelin | -0.05 | 0.753 | 0.857 |  | -0.04 | 0.814 | 0.829 |  | | 0.3 | | 0.091 | 0.174 |  | | -0.19 | | 0.274 | 0.285 |
| triglyceride | -0.04 | 0.825 | 0.857 |  | -0.06 | 0.724 | 0.829 |  | | 0.35 | | 0.043 | 0.123 |  | | -0.23 | | 0.176 | 0.222 |
| glycerophospholipid | -0.15 | 0.347 | 0.666 |  | -0.11 | 0.481 | 0.788 |  | | 0.23 | | 0.196 | 0.235 |  | | -0.33 | | 0.050 | 0.086 |

**Rho: spearman’s correlation coefficient measures the strength of association between two variables; FDR: false discovery rate**

**Table S22:** Correlation of metabolites ratios with GlycA, GlycB, CRP, and Albumin intensity value

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **GlycA** | | |  | **GlycB** | | |  | **CRP** | | |  | **Albumin** | | |
| **Feature** | **rho** | **p-value** | **FDR** |  | **rho** | **p-value** | **FDR** |  | **rho** | **p-value** | **FDR** |  | **rho** | **p-value** | **FDR** |
| Glucose/Lactate | -0.03 | 0.867 | 0.960 |  | 0.01 | 0.970 | 0.970 |  | -0.44 | 0.006 | 0.004 |  | 0.19 | 0.256 | 0.683 |
| Pyruvate/Lactate | -0.08 | 0.622 | 0.778 |  | -0.07 | 0.631 | 0.631 |  | -0.09 | 0.585 | 0.585 |  | -0.08 | 0.644 | 0.683 |
| Threonine/Glycine | -0.01 | 0.960 | 0.960 |  | -0.08 | 0.584 | 0.631 |  | -0.36 | 0.029 | 0.143 |  | 0.48 | 0.002 | 0.011 |
| Glutamine/Glutamate | -0.09 | 0.568 | 0.778 |  | -0.13 | 0.381 | 0.631 |  | -0.18 | 0.286 | 0.408 |  | 0.07 | 0.683 | 0.683 |
| 3-Hydroxybutyrate/Acetoacetate | 0.12 | 0.431 | 0.778 |  | 0.12 | 0.450 | 0.631 |  | 0.24 | 0.160 | 0.399 |  | -0.07 | 0.661 | 0.683 |
| Glutamate/Alanine | 0.11 | 0.473 | 0.778 |  | 0.12 | 0.417 | 0.631 |  | 0.17 | 0.326 | 0.408 |  | -0.13 | 0.444 | 0.683 |

**Rho: spearman’s correlation coefficient measures the strength of association between two variables; FDR: false discovery rate**

**Table S23:** Correlation of lipoproteins with GlycA, GlycB, CRP, and Albumin intensity value

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **GlycA** | | |  | **GlycB** | | |  | **CRP** | | |  | **Albumin** | | | |
| **Lipoproteins** | **rho** | **p-value** | **FDR** |  | **rho** | **p-value** | **FDR** |  | **rho** | **p-value** | **FDR** |  | **rho** | **p-value** | **FDR** |
| VLDLC (nmol/L) | 0.18 | 0.224 | 0.937 |  | -0.01 | 0.956 | 0.965 |  | 0.26 | 0.125 | 0.181 |  | -0.08 | 0.684 | 0.684 |
| IDL.C (nmol/L) | 0.06 | 0.698 | 0.957 |  | 0.1 | 0.530 | 0.927 |  | 0.42 | 0.105 | 0.049 |  | -0.57 | <0.001 | <0.001 |
| LDL.C (nmol/L) | -0.16 | 0.305 | 0.937 |  | -0.08 | 0.582 | 0.927 |  | 0.2 | 0.233 | 0.275 |  | -0.16 | 0.316 | 0.342 |
| HDL.C (nmol/L) | -0.17 | 0.278 | 0.937 |  | -0.21 | 0.175 | 0.927 |  | -0.44 | 0.007 | 0.049 |  | 0.66 | <0.001 | <0.001 |
| VLDL.TG (nmol/L) | 0.03 | 0.854 | 0.957 |  | -0.12 | 0.431 | 0.927 |  | 0.28 | 0.938 | 0.163 |  | -0.21 | 0.202 | 0.250 |
| IDL.TG (nmol/L) | 0.07 | 0.635 | 0.957 |  | 0.1 | 0.529 | 0.927 |  | 0.4 | 0.132 | 0.049 |  | -0.57 | <0.001 | <0.001 |
| LDL.TG (nmol/L) | 0.01 | 0.996 | 0.966 |  | 0.06 | 0.713 | 0.927 |  | 0.38 | 0.189 | 0.062 |  | -0.54 | <0.001 | <0.001 |
| HDL.TG (nmol/L) | 0.02 | 0.920 | 0.957 |  | -0.01 | 0.956 | 0.965 |  | 0.11 | 0.522 | 0.565 |  | -0.22 | 0.185 | 0.240 |
| VLDL.P (nmol/L) | 0.07 | 0.653 | 0.957 |  | -0.07 | 0.630 | 0.927 |  | 0.3 | 0.762 | 0.142 |  | -0.23 | 0.158 | 0.229 |
| Large.VLDL.P (nmol/L) | -0.02 | 0.872 | 0.957 |  | -0.17 | 0.256 | 0.927 |  | 0.09 | 0.582 | 0.582 |  | -0.18 | 0.285 | 0.322 |
| Medium.VLDL.P (nmol/L) | 0.17 | 0.251 | 0.937 |  | -0.08 | 0.618 | 0.927 |  | 0.17 | 0.319 | 0.361 |  | 0.12 | 0.452 | 0.470 |
| Small.VLDL.P(nmol/L) | 0.06 | 0.711 | 0.957 |  | -0.09 | 0.568 | 0.927 |  | 0.31 | 0.637 | 0.127 |  | -0.25 | 0.129 | 0.197 |
| LDLP (nmol/L) | -0.16 | 0.279 | 0.937 |  | -0.09 | 0.575 | 0.927 |  | 0.24 | 0.149 | 0.185 |  | -0.29 | 0.760 | 0.124 |
| Large.LDLP (nmol/L) | -0.03 | 0.856 | 0.957 |  | -0.04 | 0.776 | 0.961 |  | 0.33 | 0.473 | 0.112 |  | -0.18 | 0.268 | 0.317 |
| Medium.LDLP (nmol/L) | -0.09 | 0.553 | 0.957 |  | -0.02 | 0.901 | 0.965 |  | 0.27 | 0.104 | 0.169 |  | -0.31 | 0.541 | 0.108 |
| Small.LDLP (nmol/L) | -0.35 | 0.020 | 0.524 |  | -0.26 | 0.904 | 0.927 |  | 0.1 | 0.568 | 0.582 |  | -0.22 | 0.791 | 0.240 |
| HDL.P (nmol/L) | -0.16 | 0.283 | 0.937 |  | -0.19 | 0.209 | 0.927 |  | -0.42 | 0.944 | 0.049 |  | 0.67 | <0.001 | <0.001 |
| Large.HDLP (nmol/L) | 0.09 | 0.547 | 0.957 |  | -0.04 | 0.813 | 0.961 |  | -0.26 | 0.121 | 0.181 |  | 0.49 | <0.001 | <0.001 |
| Medium.HDL.P (nmol/L) | -0.05 | 0.760 | 0.957 |  | -0.11 | 0.456 | 0.927 |  | -0.31 | 0.625 | 0.127 |  | 0.37 | <0.001 | <0.001 |
| Small.HDLP (nmol/L) | -0.13 | 0.411 | 0.957 |  | -0.17 | 0.267 | 0.927 |  | -0.42 | 0.984 | 0.049 |  | 0.72 | <0.001 | <0.001 |
| VLDL.Z (nm) | 0.06 | 0.680 | 0.957 |  | 0.01 | 0.948 | 0.965 |  | -0.25 | 0.133 | 0.181 |  | 0.4 | <0.001 | <0.001 |
| LDL (nm) | 0.27 | 0.068 | 0.887 |  | 0.21 | 0.161 | 0.927 |  | 0.36 | 0.290 | 0.076 |  | -0.29 | 0.713 | 0.124 |
| HDL.Z (nm) | 0.09 | 0.559 | 0.957 |  | 0.13 | 0.398 | 0.927 |  | 0.36 | 0.286 | 0.076 |  | -0.69 | <0.001 | <0.001 |
| Non.HDL.P (nmol/L) | -0.15 | 0.324 | 0.957 |  | -0.08 | 0.587 | 0.927 |  | 0.25 | 0.143 | 0.185 |  | -0.3 | 0.634 | 0.118 |
| Total.P.HDL.P | 0.02 | 0.896 | 0.957 |  | 0.06 | 0.678 | 0.927 |  | 0.42 | 0.877 | 0.049 |  | -0.59 | <0.001 | <0.001 |
| LDL.P.HDL.P | 0.02 | 0.908 | 0.957 |  | 0.07 | 0.659 | 0.927 |  | 0.41 | 0.113 | 0.049 |  | -0.58 | <0.001 | <0.001 |

**Rho: spearman’s correlation coefficient measures the strength of association between two variables; FDR: false discovery rate**