**Supplementary Table 1**. Metabolites between the healthy control and NAFLD groups in men and women

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Healthy controls(n=71) | NAFLD (n=30) |  |  |
| **Metabolites** | Mean | SD | Mean | SD |  p BH | Group by gender |
| **Lipoprotein subclasses** |  |  |  |  |  |  |
| albumine  | 0.084  | 0.007  | 0.085  | 0.007  | 0.663  | 0.957 |
| XXL-VLDL-P  | 0.061  | 0.061  | 0.146  | 0.107  | **0.003**  | 0.388 |
| XXL-VLDL-L  | 0.012  | 0.011  | 0.025  | 0.021  | **0.014**  | 0.165 |
| XXL-VLDL-PL  | 0.002  | 0.001  | 0.003  | 0.002  | **0.023**  | 0.359 |
| XXL-VLDL-TG  | 0.008  | 0.008  | 0.018  | 0.015  | **0.008**  | 0.153 |
| XL-VLDL-P  | 0.330  | 0.334  | 0.713  | 0.484  | **0.007**  | 0.204 |
| XL-VLDL-L  | 0.036  | 0.033  | 0.072  | 0.053  | **0.010**  | 0.392 |
| XL-VLDL-PL  | 0.006  | 0.006  | 0.014  | 0.011  | **0.007**  | 0.609 |
| XL-VLDL-TG  | 0.022  | 0.021  | 0.045  | 0.034  | **0.010**  | 0.396 |
| L-VLDL-P | 2.358  | 2.125  | 4.818  | 2.840  | **0.002**  | 0.075 |
| L-VLDL-L  | 0.150  | 0.132  | 0.299  | 0.177  | **0.002**  | 0.089 |
| L-VLDL-PL  | 0.026  | 0.025  | 0.055  | 0.033  | **0.002**  | 0.126 |
| L-VLDL-C | 0.035  | 0.029  | 0.068  | 0.040  | **0.003**  | **0.007** |
| L-VLDL-CE | 0.020  | 0.015  | 0.036  | 0.021  | **0.003**  | 0.075 |
| L-VLDL-FC | 0.016  | 0.014  | 0.034  | 0.023  | **0.003**  | **0.044** |
| L-VLDL-TG | 0.090  | 0.076  | 0.185  | 0.118  | **0.002**  | **0.034** |
| M-VLDL- P | 10.21  | 6.290  | 16.35  | 7.130  | **0.001**  | 0.051 |
| M-VLDL-L  | 0.375  | 0.218  | 0.584  | 0.248  | **0.001**  | 0.100 |
| M-VLDL-PL | 0.077  | 0.043  | 0.118  | 0.047  | **0.001**  | 0.084 |
| M-VLDL-C | 0.110  | 0.056  | 0.168  | 0.065  | **0.001**  | **0.046** |
| M-VLDL-CE | 0.065  | 0.029  | 0.093  | 0.033  | **0.001**  | 0.088 |
| M-VLDL-FC | 0.046  | 0.027  | 0.075  | 0.033  | **0.001**  | **0.020** |
| M-VLDL-TG  | 0.185  | 0.121  | 0.314  | 0.153  | **0.001**  | 0.052 |
| S-VLDL-P | 22.62  | 7.984  | 30.16  | 8.186  | **0.001**  | **0.025** |
| S-VLDL-L  | 0.484  | 0.168  | 0.641  | 0.166  | **0.001**  | **0.023** |
| S-VLDL-PL | 0.113  | 0.035  | 0.145  | 0.033  | **0.001**  | **0.023** |
| S-VLDL-C  | 0.178  | 0.058  | 0.225  | 0.053  | **0.002**  | **0.031** |
| S-VLDL-FC  | 0.071  | 0.024  | 0.092  | 0.022  | **0.001**  | **0.014** |
| S-VLDL-TG  | 0.192  | 0.079  | 0.271  | 0.087  | **0.001**  | **0.033** |
| XS-VLDL-P  | 0.031  | 0.007  | 0.036  | 0.007  | **0.028**  | 0.230 |
| XS-VLDL-L  | 0.450  | 0.105  | 0.505  | 0.096  | **0.036**  | 0.216 |
| XS-VLDL-PL  | 0.133  | 0.032  | 0.144  | 0.032  | 0.182  | 0.443 |
| XS-VLDL-TG | 0.105  | 0.028  | 0.126  | 0.027  | **0.004**  | 0.053 |
| IDL-P | 0.079  | 0.017  | 0.086  | 0.017  | 0.154  | 0.472 |
| IDL-L  | 0.968  | 0.205  | 1.038  | 0.205  | 0.182  | 0.485 |
| IDL-PL  | 0.264  | 0.055  | 0.282  | 0.057  | 0.205  | 0.656 |
| IDL-C  | 0.584  | 0.125  | 0.616  | 0.128  | 0.322  | 0.534 |
| IDL-FC  | 0.182  | 0.039  | 0.187  | 0.043  | 0.627  | 0.611 |
| IDL-TG  | 0.117  | 0.027  | 0.128  | 0.026  | 0.107  | 0.186 |
| L-LDL-P  | 0.130  | 0.027  | 0.141  | 0.028  | 0.130  | 0.368 |
| L-LDL-L  | 1.154  | 0.246  | 1.251  | 0.259  | 0.135  | 0.379 |
| L-LDL-PL  | 0.286  | 0.053  | 0.308  | 0.053  | 0.122  | 0.575 |
| L-LDL-C  | 0.758  | 0.173  | 0.823  | 0.187  | 0.154  | 0.390 |
| L-LDL-CE  | 0.535  | 0.130  | 0.589  | 0.140  | 0.117  | 0.347 |
| L-LDL-FC  | 0.224  | 0.043  | 0.233  | 0.047  | 0.433  | 0.640 |
| M-LDL-P  | 0.106  | 0.023  | 0.117  | 0.024  | 0.074  | 0.404 |
| M-LDL-L  | 0.676  | 0.154  | 0.748  | 0.164  | 0.076  | 0.421 |
| M-LDL-PL  | 0.177  | 0.031  | 0.194  | 0.032  | **0.039**  | 0.522 |
| M-LDL-C  | 0.444  | 0.110  | 0.494  | 0.122  | 0.092  | 0.456 |
| M-LDL-CE  | 0.314  | 0.087  | 0.355  | 0.097  | 0.082  | 0.428 |
| S-LDL-P  | 0.127  | 0.027  | 0.142  | 0.029  | **0.028**  | 0.138 |
| S-LDL-L  | 0.446  | 0.104  | 0.507  | 0.112  | **0.027**  | 0.146 |
| S-LDL-C  | 0.282  | 0.069  | 0.320  | 0.080  | **0.039**  | 0.150 |
| XL-HDL-P  | 0.393  | 0.167  | 0.286  | 0.092  | **0.001**  | 0.886 |
| XL-HDL-L  | 0.481  | 0.192  | 0.367  | 0.108  | **0.003**  | 0.831 |
| XL-HDL-PL  | 0.234  | 0.107  | 0.161  | 0.061  | **0.001**  | 0.828 |
| XL-HDL-C  | 0.244  | 0.101  | 0.194  | 0.055  | **0.009**  | 0.722 |
| XL-HDL-CE  | 0.179  | 0.071  | 0.143  | 0.040  | **0.009**  | 0.414 |
| XL-HDL-FC  | 0.063  | 0.028  | 0.046  | 0.015  | **0.002**  | 0.990 |
| XL-HDL-TG  | 0.013  | 0.004  | 0.013  | 0.003  | 0.565  | 0.280 |
| L-HDL-P  | 1.034  | 0.396  | 0.780  | 0.307  | **0.010**  | 0.988 |
| L-HDL-L  | 0.801  | 0.317  | 0.592  | 0.240  | **0.008**  | 0.987 |
| L-HDL-PL  | 0.389  | 0.137  | 0.305  | 0.114  | **0.014**  | 0.996 |
| L-HDL-C  | 0.386  | 0.173  | 0.266  | 0.124  | **0.005**  | 0.933 |
| L-HDL-CE  | 0.300  | 0.133  | 0.211  | 0.096  | **0.007**  | 0.933 |
| L-HDL-FC  | 0.086  | 0.040  | 0.054  | 0.029  | **0.002**  | 0.864 |
| M-HDL-P  | 1.594  | 0.288  | 1.679  | 0.308  | 0.266  | 0.567 |
| M-HDL-L  | 0.851  | 0.160  | 0.889  | 0.166  | 0.366  | 0.580 |
| M-HDL-PL  | 0.396  | 0.068  | 0.413  | 0.076  | 0.334  | 0.612 |
| M-HDL-C  | 0.419  | 0.091  | 0.430  | 0.086  | 0.626  | 0.577 |
| M-HDL-CE  | 0.339  | 0.073  | 0.347  | 0.068  | 0.631  | 0.591 |
| M-HDL-FC  | 0.079  | 0.018  | 0.080  | 0.019  | 0.663  | 0.586 |
| S-HDL-P  | 3.929  | 0.379  | 4.160  | 0.342  | **0.016**  | 0.676 |
| S-HDL-L  | 1.037  | 0.114  | 1.101  | 0.107  | **0.027**  | 0.801 |
| S-HDL-TG  | 0.040  | 0.012  | 0.048  | 0.012  | **0.013**  | 0.715 |
| VLDL-TG | 0.568  | 0.309  | 0.891  | 0.371  | **0.001**  | 0.058 |
| LDL-C  | 1.483  | 0.350  | 1.640  | 0.385  | 0.094  | 0.271 |
| HDL-C  | 1.509  | 0.339  | 1.327  | 0.244  | **0.026**  | 0.963 |
| Serum-C  | 4.094  | 0.717  | 4.249  | 0.671  | 0.396  | 0.329 |
| VLDL-D | 35.77  | 1.194  | 36.99  | 1.334  | **0.001**  | **0.040** |
| LDL-D  | 23.51  | 0.160  | 23.45  | 0.149  | 0.158  | 0.161 |
| HDL-D  | 10.04  | 0.289  | 9.839  | 0.165  | **0.001**  | 0.812 |
| VLDL-TG-eFR | 0.528  | 0.254  | 0.804  | 0.315  | **0.001**  | 0.072 |
| IDL-C-eFR | 0.158  | 0.052  | 0.208  | 0.060  | **0.001**  | 0.098 |
| LDL-C-eFR  | 2.430  | 0.453  | 2.526  | 0.469  | 0.413  | 0.554 |
| HDL2-C  | 1.006  | 0.320  | 0.818  | 0.214  | **0.014**  | 0.811 |
| HDL3-C  | 0.503  | 0.042  | 0.509  | 0.043  | 0.582  | 0.205 |
| Apolipoprotein A1a | 1.552  | 0.245  | 1.483  | 0.187  | 0.240  | 0.342 |
| Apolipoprotein Ba | 0.752  | 0.152  | 0.878  | 0.162  | **0.002**  | 0.142 |
| ApoB/ApoA1 | 0.493  | 0.117  | 0.598  | 0.118  | **0.001**  | 0.415 |
| **Lipid extract constituents** |  |  |  |  |  |  |
| Mobile lipids Ch2 | 18.89  | 6.810  | 25.94  | 8.751  | **0.000** | 0.073 |
| Mobile lipids Ch3 | 7.314  | 1.480  | 8.589  | 1.738  | **0.000**  | **0.038** |
| Omega7and 9 fatty acids  | 5.194  | 1.209  | 6.349  | 1.519  | **0.001**  | 0.106 |
| MUFA | 2.339  | 0.662  | 2.972  | 0.773  | **0.001**  | 0.087 |
| Omega7and9/ total fatty acid ratio | 60.08  | 3.150  | 63.16  | 4.780  | **0.011**  | 0.062 |
| Triglycerides/phosphoglycerides | 1.189  | 0.453  | 1.644  | 0.654  | **0.007**  | 0.503 |
| Esterified cholesterol  | 2.953  | 0.517  | 3.070  | 0.499  | 0.389  | 0.294 |
| Free cholesterol  | 1.140  | 0.212  | 1.171  | 0.197  | 0.572  | 0.524 |
| Omega3 fatty acids  | 0.413  | 0.166  | 0.444  | 0.187  | 0.493  | 0.294 |
| Omega6 fatty acids  | 2.994  | 0.444  | 3.181  | 0.503  | 0.124  | 0.625 |
| Total fatty acids | 8.61 | 1.69 | 10.04 | 1.91 | **0.001** | 0.092 |
| Total phosphoglycerides  | 0.648  | 0.143  | 0.692  | 0.109  | 0.205  | 0.297 |
| Total phosphocholines  | 1.583  | 0.300  | 1.652  | 0.235  | 0.354  | 0.344 |
| Sphingomyelines  | 0.213  | 0.046  | 0.215  | 0.043  | 0.785  | 0.828 |
| Omega3/total fatty acid ratio | 4.734  | 1.417  | 4.419  | 1.599  | 0.413  | 0.598 |
| Omega6/total fatty acid ratio | 35.18  | 3.225  | 32.42  | 4.861  | **0.023**  | 0.054 |
| CH2 in total fatty acids | 9.547  | 0.200  | 9.629  | 0.210  | 0.124  | 0.575 |
| Linoleic acid  | 2.525  | 0.402  | 2.626  | 0.491  | 0.377  | 0.472 |
| Other polyunsaturated fatty acids  | 1.797  | 0.577  | 1.994  | 0.526  | 0.182  | 0.313 |
| Docosahexaenoic acid  | 1.286  | 0.090  | 1.241  | 0.109  | 0.074  | 0.216 |
| fatty acid length | 17.98  | 0.206  | 17.92  | 0.197  | 0.334  | 0.638 |
| **Low-molecular weight metabolites** |  |  |  |  |  |  |
| Betahydroxybutyrate  | 0.052  | 0.049  | 0.047  | 0.035  | 0.695  | 0.865 |
| Acetate | 0.051  | 0.069  | 0.041  | 0.012  | **0.045**  | 0.333 |
| Acetoacetate | 0.039  | 0.019  | 0.040  | 0.022  | **0.003**  | 0.453 |
| Alanine | 0.379  | 0.052  | 0.408  | 0.063  | **0.002**  | 0.391 |
| Citrate | 0.100  | 0.018  | 0.105  | 0.017  | 0.276  | 0.740 |
| Creatinine | 0.057  | 0.010  | 0.059  | 0.015  | 0.614  | 0.119 |
| Glutamine | 0.556  | 0.055  | 0.536  | 0.062  | 0.182  | 0.715 |
| Glycerol | 0.060  | 0.021  | 0.082  | 0.028  | **0.001**  | **0.039** |
| Glycine | 0.278  | 0.062  | 0.247  | 0.042  | **0.033**  | 0.152 |
| Orosomucoid | 1.219  | 0.158  | 1.374  | 0.174  | **0.001**  | 0.140 |
| Histidine | 0.051  | 0.007  | 0.053  | 0.009  | 0.238  | 0.885 |
| Isoleucine | 0.042  | 0.010  | 0.054  | 0.011  | **0.000**  | 0.387 |
| Leucine | 0.066  | 0.012  | 0.080  | 0.013  | **0.001**  | 0.291 |
| Valine | 0.171  | 0.030  | 0.196  | 0.035  | **0.003**  | 0.785 |
| Phenylalanine | 0.063  | 0.008  | 0.068  | 0.008  | **0.016**  | 0.414 |
| Pyruvate | 0.068  | 0.017  | 0.078  | 0.017  | **0.030**  | 0.745 |
| Tyrosine | 0.044  | 0.008  | 0.051  | 0.010  | **0.003**  | 0.172 |
| Urea | 0.058  | 0.023  | 0.054  | 0.024  | 0.500  | 0.610 |
| Lactate | 0.906  | 0.225  | 1.000  | 0.299  | 0.147  | 0.681 |

Mean (SD) concentrations of metabolites assayed in the present study. Concentrations are in mmol/l unless stated otherwise. P-values are for 2-tailed t-tests comparing concentrations between healthy controls and NAFLD (non-alcohol fatty liver disease) groups adjusted for multiple comparisons using Benjamin-Hochberg correction. Abbreviations: VLDL: very-low-density lipoprotein; IDL: intermediate –density lipoprotein; LDL: low-density lipoprotein; HDL: high-density lipoprotein; XXL: extremely large; XL: very large; L: large; M: medium; S: small; XS: very small; L: total protein lipids; PL: phospholipids; C: cholesterol; CE: cholesterol esters; FC: free cholesterol; TG: triglycerides; D: mean diameter; eFR=values estimated with the extended friedewald method; Bis/DB: bisallylic groups per double bond; a=g/l. Significant differences are marked in bold.