S4 Table. Abbreviations and full names of metabolites

Abbreviation Full name Unit

|  |  |  |
| --- | --- | --- |
| Alb | Albumin | signal area |
| XXL\_VLDL\_PL | Phospholipids in chylomicrons and extremely large VLDL | mmol/l |
| XXL\_VLDL\_L | Total lipids in chylomicrons and extremely large VLDL | mmol/l |
| XXL\_VLDL\_P | Concentration of chylomicrons and extremely large VLDL particles | mol/l |
| XL\_VLDL\_PL | Phospholipids in very large VLDL | mmol/l |
| XL\_VLDL\_TG | Triglycerides in very large VLDL | mmol/l |
| XL\_VLDL\_L | Total lipids in very large VLDL | mmol/l |
| XL\_VLDL\_P | Concentration of very large VLDL particles | mol/l |
| L\_VLDL\_C | Total cholesterol in large VLDL | mmol/l |
| L\_VLDL\_FC | Free cholesterol in large VLDL | mmol/l |
| L\_VLDL\_PL | Phospholipids in large VLDL | mmol/l |
| L\_VLDL\_TG | Triglycerides in large VLDL | mmol/l |
| L\_VLDL\_CE | Cholesterol esters in large VLDL | mmol/l |
| L\_VLDL\_L | Total lipids in large VLDL | mmol/l |
| L\_VLDL\_P | Concentration of large VLDL particles | mol/l |
| M\_VLDL\_C | Total cholesterol in medium VLDL | mmol/l |
| M\_VLDL\_FC | Free cholesterol in medium VLDL | mmol/l |
| M\_VLDL\_PL | Phospholipids in medium VLDL | mmol/l |
| M\_VLDL\_TG | Triglycerides in medium VLDL | mmol/l |
| M\_VLDL\_CE | Cholesterol esters in medium VLDL | mmol/l |
| M\_VLDL\_L | Total lipids in medium VLDL | mmol/l |
| M\_VLDL\_P | Concentration of medium VLDL particles | mol/l |
| S\_VLDL\_C | Total cholesterol in small VLDL | mmol/l |
| S\_VLDL\_FC | Free cholesterol in small VLDL | mmol/l |
| S\_VLDL\_PL | Phospholipids in small VLDL | mmol/l |
| S\_VLDL\_TG | Triglycerides in small VLDL | mmol/l |
| S\_VLDL\_L | Total lipids in small VLDL | mmol/l |
| S\_VLDL\_P | Concentration of small VLDL particles | mol/l |
| XS\_VLDL\_PL | Phospholipids in very small VLDL | mmol/l |
| XS\_VLDL\_TG | Triglycerides in very small VLDL | mmol/l |
| XS\_VLDL\_L | Total lipids in very small VLDL | mmol/l |
| XS\_VLDL\_P | Concentration of very small VLDL particles | mol/l |
| IDL\_FC | Free cholesterol in IDL | mmol/l |
| IDL\_PL | Phospholipids in IDL | mmol/l |
| IDL\_L | Total lipids in IDL | mmol/l |
| IDL\_P | Concentration of IDL particles | mol/l |
| L\_LDL\_C | Total cholesterol in large LDL | mmol/l |
| L\_LDL\_FC | Free cholesterol in large LDL | mmol/l |
| L\_LDL\_PL | Phospholipids in large LDL | mmol/l |
| L\_LDL\_CE | Cholesterol esters in large LDL | mmol/l |
| L\_LDL\_L | Total lipids in large LDL | mmol/l |
| L\_LDL\_P | Concentration of large LDL particles | mol/l |
| M\_LDL\_C | Total cholesterol in medium LDL | mmol/l |
| M\_LDL\_PL | Phospholipids in medium LDL | mmol/l |
| M\_LDL\_CE | Cholesterol esters in medium LDL | mmol/l |
| M\_LDL\_L | Total lipids in medium LDL | mmol/l |
| M\_LDL\_P | Concentration of medium LDL particles | mol/l |
| S\_LDL\_C | Total cholesterol in small LDL | mmol/l |
| S\_LDL\_L | Total lipids in small LDL | mmol/l |
| S\_LDL\_P | Concentration of small LDL particles | mol/l |
| XL\_HDL\_C | Total cholesterol in very large HDL | mmol/l |
| XL\_HDL\_FC | Free cholesterol in very large HDL | mmol/l |
| XL\_HDL\_PL | Phospholipids in very large HDL | mmol/l |
| XL\_HDL\_TG | Triglycerides in very large HDL | mmol/l |
| XL\_HDL\_CE | Cholesterol esters in very large HDL | mmol/l |
| XL\_HDL\_L | Total lipids in very large HDL | mmol/l |
| XL\_HDL\_P | Concentration of very large HDL particles | mol/l |
| L\_HDL\_C | Total cholesterol in large HDL | mmol/l |
| L\_HDL\_FC | Free cholesterol in large HDL | mmol/l |
| L\_HDL\_PL | Phospholipids in large HDL | mmol/l |
| L\_HDL\_CE | Cholesterol esters in large HDL | mmol/l |
| L\_HDL\_L | Total lipids in large HDL | mmol/l |
| L\_HDL\_P | Concentration of large HDL particles | mol/l |
| M\_HDL\_C | Total cholesterol in medium HDL | mmol/l |
| M\_HDL\_FC | Free cholesterol in medium HDL | mmol/l |
| M\_HDL\_PL | Phospholipids in medium HDL | mmol/l |
| M\_HDL\_CE | Cholesterol esters in medium HDL | mmol/l |
| M\_HDL\_L | Total lipids in medium HDL | mmol/l |
| M\_HDL\_P | Concentration of medium HDL particles | mol/l |
| S\_HDL\_TG | Triglycerides in small HDL | mmol/l |
| S\_HDL\_L | Total lipids in small HDL | mmol/l |
| S\_HDL\_P | Concentration of small HDL particles | mol/l |
| XXL\_VLDL\_TG | Triglycerides in chylomicrons and extremely large VLDL | mmol/l |
| VLDL\_TG | Triglycerides in VLDL | mmol/l |
| IDL\_TG | Triglycerides in IDL | mmol/l |
| IDL\_C | Total cholesterol in IDL | mmol/l |
| LDL\_C | Total cholesterol in LDL | mmol/l |
| HDL\_C | Total cholesterol in HDL | mmol/l |
| Serum\_TG | Serum total triglycerides | mmol/l |
| Serum\_C | Serum total cholesterol | mmol/l |
| VLDL\_D | Mean diameter for VLDL particles | nm |
| LDL\_D | Mean diameter for LDL particles | nm |
| HDL\_D | Mean diameter for HDL particles | nm |
| VLDL\_TG\_eFR | Triglycerides in VLDL \* | mmol/l |
| IDL\_C\_eFR | Total cholesterol in IDL \* | mmol/l |
| LDL\_C\_eFR | Total cholesterol in LDL \* | mmol/l |
| HDL2\_C | Total cholesterol in HDL2 \* | mmol/l |
| ApoA1 | Apolipoprotein A-I \* | g/l |
| ApoB | Apolipoprotein B \* | g/l |
| ApoBtoApoA1 | Apolipoprotein B by apolipoprotein A-I \* |  |
| HDL3\_C | Total cholesterol in HDL3 \* | mmol/l |
| bOHBut | 3-hydroxybutyrate | mmol/l |
| Ace | Acetate | mmol/l |
| AcAce | Acetoacetate | mmol/l |
| Ala | Alanine | mmol/l |
| MobCH2 | CH2 groups of mobile lipids | mmol/l |
| MobCH3 | CH3 groups of mobile lipids | mmol/l |
| Cit | Citrate | mmol/l |
| Crea | Creatinine | mmol/l |
| MobCH | Double bond protons of mobile lipids | mmol/l |
| Glc | Glucose | mmol/l |
| Gln | Glutamine | mmol/l |
| Glol | Glycerol | mmol/l |
| Gly | Glycine | mmol/l |
| Gp | Glycoprotein acetyls, mainly a1-acid glycoprotein | mmol/l |
| His | Histidine | mmol/l |
| Ile | Isoleucine | mmol/l |
| Lac | Lactate | mmol/l |
| Leu | Leucine | mmol/l |
| Phe | Phenylalanine | mmol/l |
| Pyr | Pyruvate | mmol/l |
| Tyr | Tyrosine | mmol/l |
| Urea | Urea | mmol/l |
| Val | Valine | mmol/l |
| EstC | Esterified cholesterol | mmol/l |
| FreeC | Free cholesterol | mmol/l |
| FAw3 | Omega-3 fatty acids | mmol/l |
| FAw6 | Omega-6 fatty acids | mmol/l |
| FAw79S | Omega-7, omega-9 and saturated fatty acids | mmol/l |
| TotFA | Total fatty acids | mmol/l |
| LA | 18:2, linoleic acid | mmol/l |
| otPUFA | Other polyunsaturated fatty acids than 18:2 | \*\* |
| DHA | 22:6, docosahexaenoic acid | mmol/l |
| MUFA | Monounsaturated fatty acids; 16:1, 18:1 | mmol/l |
| TotPG | Total phosphoglycerides | mmol/l |
| PC | Phosphatidylcholine and other cholines | mmol/l |
| SM | Sphingomyelins | mmol/l |
| FAw3toFA | Ratio of omega-3 fatty acids to total fatty acids | % |
| FAw6toFA | Ratio of omega-6 fatty acids to total fatty acids | % |
| FAw79StoFA | Ratio of omega-7, omega-9 and saturated fatty acids to total fatty acids | % |
| CH2inFA | Average number of methylene groups in a fatty acid chain |  |
| TGtoPG | Ratio of triglycerides to phosphoglycerides |  |
| CH2toDB | Average number of methylene groups per a double bond |  |
| DBinFA | Average number of double bonds in a fatty acid chain |  |
| BIStoDB | Ratio of bisallylic groups to double bonds |  |
| BIStoFA | Ratio of bisallylic groups to total fatty acids |  |
| FALen | Description of average fatty acid chain length, not actual carbon number |  |

\*Values estimated with the Extended Friedewald method.