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.