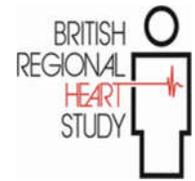


Q20 Metabolite data

1998 - 2000



Methods

A high-throughput serum nuclear magnetic resonance (NMR) metabolomics platform was used to quantify >200 metabolite markers from unfrozen serum samples that represent a broad molecular signature of systemic metabolism. The metabolites were measured in a single experimental setup that allows for the simultaneous quantification of fatty acid composition (including monounsaturated fatty acids, saturated fatty acids, and polyunsaturated fatty acids), lipoprotein subclasses, α -1 acid glycoprotein, amino acids, glycolysis-related measures, and ketone bodies (Nightingale Health Ltd., Helsinki, Finland). Applications of this high-throughput platform have been described elsewhere [1,2,3]

1. Soininen P, Kangas AJ, Wurtz P, Tukiainen T, Tynkynen T, Laatikainen R. High-throughput serum NMR metabolomics for cost-effective holistic studies on systemic metabolism. *Analyst*. 2009;134:1781–1785.
2. Soininen P, Kangas AJ, Wurtz P, Suna T, Ala-Korpela M. Quantitative serum nuclear magnetic resonance metabolomics in cardiovascular epidemiology and genetics. *Circ Cardiovasc Genet*. 2015;8:192–206.
3. Wurtz P, Kangas AJ, Soininen P, Lawlor DA, Davey Smith G, Ala-Korpela M. Quantitative serum nuclear magnetic resonance metabolomics in large-scale epidemiology: a primer on -omic technologies. *Am J Epidemiol*. 2017;186:1084–1096.

LIST OF Q20(1998-2000) METABOLITES	BRHS VARIABLE NAME	Data access
Low glutamine / high glutamate	q20metab_Low_high_glutamate	Yes
Low protein content	q20metab_Low_protein	Yes
High ethanol	q20metab_High_ethanol	Yes
Concentration of chylomicrons and extremely large VLDL particles	q20metab_XXL_VLDL_P	Yes
Total lipids in chylomicrons and extremely large VLDL	q20metab_XXL_VLDL_L	Yes
Phospholipids in chylomicrons and extremely large VLDL	q20metab_XXL_VLDL_PL	Yes
Total cholesterol in chylomicrons and extremely large VLDL	q20metab_XXL_VLDL_C	Yes
Cholesterol esters in chylomicrons and extremely large VLDL	q20metab_XXL_VLDL_CE	Yes
Free cholesterol in chylomicrons and extremely large VLDL	q20metab_XXL_VLDL_FC	Yes
Triglycerides in chylomicrons and extremely large VLDL	q20metab_XXL_VLDL_TG	Yes
Concentration of very large VLDL particles	q20metab_XL_VLDL_P	Yes
Total lipids in very large VLDL	q20metab_XL_VLDL_L	Yes
Phospholipids in very large VLDL	q20metab_XL_VLDL_PL	Yes
Total cholesterol in very large VLDL	q20metab_XL_VLDL_C	Yes
Cholesterol esters in very large VLDL	q20metab_XL_VLDL_CE	Yes
Free cholesterol in very large VLDL	q20metab_XL_VLDL_FC	Yes
Triglycerides in very large VLDL	q20metab_XL_VLDL_TG	Yes
Concentration of large VLDL particles	q20metab_L_VLDL_P	Yes
Total lipids in large VLDL	q20metab_L_VLDL_L	Yes
Phospholipids in large VLDL	q20metab_L_VLDL_PL	Yes
Total cholesterol in large VLDL	q20metab_L_VLDL_C	Yes
Cholesterol esters in large VLDL	q20metab_L_VLDL_CE	Yes
Free cholesterol in large VLDL	q20metab_L_VLDL_FC	Yes
Triglycerides in large VLDL	q20metab_L_VLDL_TG	Yes
Concentration of medium VLDL particles	q20metab_M_VLDL_P	Yes
Total lipids in medium VLDL	q20metab_M_VLDL_L	Yes
Phospholipids in medium VLDL	q20metab_M_VLDL_PL	Yes
Total cholesterol in medium VLDL	q20metab_M_VLDL_C	Yes
Cholesterol esters in medium VLDL	q20metab_M_VLDL_CE	Yes
Free cholesterol in medium VLDL	q20metab_M_VLDL_FC	Yes
Triglycerides in medium VLDL	q20metab_M_VLDL_TG	Yes
Concentration of small VLDL particles	q20metab_S_VLDL_P	Yes
Total lipids in small VLDL	q20metab_S_VLDL_L	Yes
Phospholipids in small VLDL	q20metab_S_VLDL_PL	Yes
Total cholesterol in small VLDL	q20metab_S_VLDL_C	Yes
Cholesterol esters in small VLDL	q20metab_S_VLDL_CE	Yes
Free cholesterol in small VLDL	q20metab_S_VLDL_FC	Yes
Triglycerides in small VLDL	q20metab_S_VLDL_TG	Yes
Concentration of very small VLDL particles	q20metab_XS_VLDL_P	Yes
Total lipids in very small VLDL	q20metab_XS_VLDL_L	Yes
Phospholipids in very small VLDL	q20metab_XS_VLDL_PL	Yes
Total cholesterol in very small VLDL	q20metab_XS_VLDL_C	Yes
Cholesterol esters in very small VLDL	q20metab_XS_VLDL_CE	Yes
Free cholesterol in very small VLDL	q20metab_XS_VLDL_FC	Yes
Triglycerides in very small VLDL	q20metab_XS_VLDL_TG	Yes
Concentration of IDL particles	q20metab_IDL_P	Yes
Total lipids in IDL	q20metab_IDL_L	Yes
Phospholipids in IDL	q20metab_IDL_PL	Yes

Total cholesterol in IDL	q20metab_IDL_C	Yes
Cholesterol esters in IDL	q20metab_IDL_CE	Yes
Free cholesterol in IDL	q20metab_IDL_FC	Yes
Triglycerides in IDL	q20metab_IDL_TG	Yes
Concentration of large LDL particles	q20metab_L_LDL_P	Yes
Total lipids in large LDL	q20metab_L_LDL_L	Yes
Phospholipids in large LDL	q20metab_L_LDL_PL	Yes
Total cholesterol in large LDL	q20metab_L_LDL_C	Yes
Cholesterol esters in large LDL	q20metab_L_LDL_CE	Yes
Free cholesterol in large LDL	q20metab_L_LDL_FC	Yes
Triglycerides in large LDL	q20metab_L_LDL_TG	Yes
Concentration of medium LDL particles	q20metab_M_LDL_P	Yes
Total lipids in medium LDL	q20metab_M_LDL_L	Yes
Phospholipids in medium LDL	q20metab_M_LDL_PL	Yes
Total cholesterol in medium LDL	q20metab_M_LDL_C	Yes
Cholesterol esters in medium LDL	q20metab_M_LDL_CE	Yes
Free cholesterol in medium LDL	q20metab_M_LDL_FC	Yes
Triglycerides in medium LDL	q20metab_M_LDL_TG	Yes
Concentration of small LDL particles	q20metab_S_LDL_P	Yes
Total lipids in small LDL	q20metab_S_LDL_L	Yes
Phospholipids in small LDL	q20metab_S_LDL_PL	Yes
Total cholesterol in small LDL	q20metab_S_LDL_C	Yes
Cholesterol esters in small LDL	q20metab_S_LDL_CE	Yes
Free cholesterol in small LDL	q20metab_S_LDL_FC	Yes
Triglycerides in small LDL	q20metab_S_LDL_TG	Yes
Concentration of very large HDL particles	q20metab_XL_HDL_P	Yes
Total lipids in very large HDL	q20metab_XL_HDL_L	Yes
Phospholipids in very large HDL	q20metab_XL_HDL_PL	Yes
Total cholesterol in very large HDL	q20metab_XL_HDL_C	Yes
Cholesterol esters in very large HDL	q20metab_XL_HDL_CE	Yes
Free cholesterol in very large HDL	q20metab_XL_HDL_FC	Yes
Triglycerides in very large HDL	q20metab_XL_HDL_TG	Yes
Concentration of large HDL particles	q20metab_L_HDL_P	Yes
Total lipids in large HDL	q20metab_L_HDL_L	Yes
Phospholipids in large HDL	q20metab_L_HDL_PL	Yes
Total cholesterol in large HDL	q20metab_L_HDL_C	Yes
Cholesterol esters in large HDL	q20metab_L_HDL_CE	Yes
Free cholesterol in large HDL	q20metab_L_HDL_FC	Yes
Triglycerides in large HDL	q20metab_L_HDL_TG	Yes
Concentration of medium HDL particles	q20metab_M_HDL_P	Yes
Total lipids in medium HDL	q20metab_M_HDL_L	Yes
Phospholipids in medium HDL	q20metab_M_HDL_PL	Yes
Total cholesterol in medium HDL	q20metab_M_HDL_C	Yes
Cholesterol esters in medium HDL	q20metab_M_HDL_CE	Yes
Free cholesterol in medium HDL	q20metab_M_HDL_FC	Yes
Triglycerides in medium HDL	q20metab_M_HDL_TG	Yes
Concentration of small HDL particles	q20metab_S_HDL_P	Yes
Total lipids in small HDL	q20metab_S_HDL_L	Yes
Phospholipids in small HDL	q20metab_S_HDL_PL	Yes
Total cholesterol in small HDL	q20metab_S_HDL_C	Yes
Cholesterol esters in small HDL	q20metab_S_HDL_CE	Yes

Free cholesterol in small HDL	q20metab_S_HDL_FC	Yes
Triglycerides in small HDL	q20metab_S_HDL_TG	Yes
Phospholipids to total lipids ratio in chylomicrons and extremely large VLDL	q20metab_XXL_VLDL_PL_pcent	Yes
Total cholesterol to total lipids ratio in chylomicrons and extremely large VLDL	q20metab_XXL_VLDL_C_pcent	Yes
Cholesterol esters to total lipids ratio in chylomicrons and extremely large VLDL	q20metab_XXL_VLDL_CE_pcent	Yes
Free cholesterol to total lipids ratio in chylomicrons and extremely large VLDL	q20metab_XXL_VLDL_FC_pcent	Yes
Triglycerides to total lipids ratio in chylomicrons and extremely large VLDL	q20metab_XXL_VLDL_TG_pcent	Yes
Phospholipids to total lipids ratio in very large VLDL	q20metab_XL_VLDL_PL_pcent	Yes
Total cholesterol to total lipids ratio in very large VLDL	q20metab_XL_VLDL_C_pcent	Yes
Cholesterol esters to total lipids ratio in very large VLDL	q20metab_XL_VLDL_CE_pcent	Yes
Free cholesterol to total lipids ratio in very large VLDL	q20metab_XL_VLDL_FC_pcent	Yes
Triglycerides to total lipids ratio in very large VLDL	q20metab_XL_VLDL_TG_pcent	Yes
Phospholipids to total lipids ratio in large VLDL	q20metab_L_VLDL_PL_pcent	Yes
Total cholesterol to total lipids ratio in large VLDL	q20metab_L_VLDL_C_pcent	Yes
Cholesterol esters to total lipids ratio in large VLDL	q20metab_L_VLDL_CE_pcent	Yes
Free cholesterol to total lipids ratio in large VLDL	q20metab_L_VLDL_FC_pcent	Yes
Triglycerides to total lipids ratio in large VLDL	q20metab_L_VLDL_TG_pcent	Yes
Phospholipids to total lipids ratio in medium VLDL	q20metab_M_VLDL_PL_pcent	Yes
Total cholesterol to total lipids ratio in medium VLDL	q20metab_M_VLDL_C_pcent	Yes
Cholesterol esters to total lipids ratio in medium VLDL	q20metab_M_VLDL_CE_pcent	Yes
Free cholesterol to total lipids ratio in medium VLDL	q20metab_M_VLDL_FC_pcent	Yes
Triglycerides to total lipids ratio in medium VLDL	q20metab_M_VLDL_TG_pcent	Yes
Phospholipids to total lipids ratio in small VLDL	q20metab_S_VLDL_PL_pcent	Yes
Total cholesterol to total lipids ratio in small VLDL	q20metab_S_VLDL_C_pcent	Yes
Cholesterol esters to total lipids ratio in small VLDL	q20metab_S_VLDL_CE_pcent	Yes
Free cholesterol to total lipids ratio in small VLDL	q20metab_S_VLDL_FC_pcent	Yes
Triglycerides to total lipids ratio in small VLDL	q20metab_S_VLDL_TG_pcent	Yes
Phospholipids to total lipids ratio in very small VLDL	q20metab_XS_VLDL_PL_pcent	Yes
Total cholesterol to total lipids ratio in very small VLDL	q20metab_XS_VLDL_C_pcent	Yes
Cholesterol esters to total lipids ratio in very small VLDL	q20metab_XS_VLDL_CE_pcent	Yes
Free cholesterol to total lipids ratio in very small VLDL	q20metab_XS_VLDL_FC_pcent	Yes
Triglycerides to total lipids ratio in very small VLDL	q20metab_XS_VLDL_TG_pcent	Yes
Phospholipids to total lipids ratio in IDL	q20metab_IDL_PL_pcent	Yes
Total cholesterol to total lipids ratio in IDL	q20metab_IDL_C_pcent	Yes
Cholesterol esters to total lipids ratio in IDL	q20metab_IDL_CE_pcent	Yes
Free cholesterol to total lipids ratio in IDL	q20metab_IDL_FC_pcent	Yes
Triglycerides to total lipids ratio in IDL	q20metab_IDL_TG_pcent	Yes
Phospholipids to total lipids ratio in large LDL	q20metab_L_LDL_PL_pcent	Yes
Total cholesterol to total lipids ratio in large LDL	q20metab_L_LDL_C_pcent	Yes
Cholesterol esters to total lipids ratio in large LDL	q20metab_L_LDL_CE_pcent	Yes
Free cholesterol to total lipids ratio in large LDL	q20metab_L_LDL_FC_pcent	Yes
Triglycerides to total lipids ratio in large LDL	q20metab_L_LDL_TG_pcent	Yes
Phospholipids to total lipids ratio in medium LDL	q20metab_M_LDL_PL_pcent	Yes
Total cholesterol to total lipids ratio in medium LDL	q20metab_M_LDL_C_pcent	Yes
Cholesterol esters to total lipids ratio in medium LDL	q20metab_M_LDL_CE_pcent	Yes
Free cholesterol to total lipids ratio in medium LDL	q20metab_M_LDL_FC_pcent	Yes
Triglycerides to total lipids ratio in medium LDL	q20metab_M_LDL_TG_pcent	Yes
Phospholipids to total lipids ratio in small LDL	q20metab_S_LDL_PL_pcent	Yes
Total cholesterol to total lipids ratio in small LDL	q20metab_S_LDL_C_pcent	Yes
Cholesterol esters to total lipids ratio in small LDL	q20metab_S_LDL_CE_pcent	Yes
Free cholesterol to total lipids ratio in small LDL	q20metab_S_LDL_FC_pcent	Yes

Triglycerides to total lipids ratio in small LDL	q20metab_S_LDL_TG_pcent	Yes
Phospholipids to total lipids ratio in very large HDL	q20metab_XL_HDL_PL_pcent	Yes
Total cholesterol to total lipids ratio in very large HDL	q20metab_XL_HDL_C_pcent	Yes
Cholesterol esters to total lipids ratio in very large HDL	q20metab_XL_HDL_CE_pcent	Yes
Free cholesterol to total lipids ratio in very large HDL	q20metab_XL_HDL_FC_pcent	Yes
Triglycerides to total lipids ratio in very large HDL	q20metab_XL_HDL_TG_pcent	Yes
Phospholipids to total lipids ratio in large HDL	q20metab_L_HDL_PL_pcent	Yes
Total cholesterol to total lipids ratio in large HDL	q20metab_L_HDL_C_pcent	Yes
Cholesterol esters to total lipids ratio in large HDL	q20metab_L_HDL_CE_pcent	Yes
Free cholesterol to total lipids ratio in large HDL	q20metab_L_HDL_FC_pcent	Yes
Triglycerides to total lipids ratio in large HDL	q20metab_L_HDL_TG_pcent	Yes
Phospholipids to total lipids ratio in medium HDL	q20metab_M_HDL_PL_pcent	Yes
Total cholesterol to total lipids ratio in medium HDL	q20metab_M_HDL_C_pcent	Yes
Cholesterol esters to total lipids ratio in medium HDL	q20metab_M_HDL_CE_pcent	Yes
Free cholesterol to total lipids ratio in medium HDL	q20metab_M_HDL_FC_pcent	Yes
Triglycerides to total lipids ratio in medium HDL	q20metab_M_HDL_TG_pcent	Yes
Phospholipids to total lipids ratio in small HDL	q20metab_S_HDL_PL_pcent	Yes
Total cholesterol to total lipids ratio in small HDL	q20metab_S_HDL_C_pcent	Yes
Cholesterol esters to total lipids ratio in small HDL	q20metab_S_HDL_CE_pcent	Yes
Free cholesterol to total lipids ratio in small HDL	q20metab_S_HDL_FC_pcent	Yes
Triglycerides to total lipids ratio in small HDL	q20metab_S_HDL_TG_pcent	Yes
Mean diameter for VLDL particles	q20metab_VLDL_D	Yes
Mean diameter for LDL particles	q20metab_LDL_D	Yes
Mean diameter for HDL particles	q20metab_HDL_D	Yes
Serum total cholesterol	q20metab_Serum_C	Yes
Total cholesterol in VLDL	q20metab_VLDL_C	Yes
Remnant cholesterol (non-HDL, non-LDL -cholesterol)	q20metab_Remnant_C	Yes
Total cholesterol in LDL	q20metab_LDL_C	Yes
Total cholesterol in HDL	q20metab_HDL_C	Yes
Total cholesterol in HDL2	q20metab_HDL2_C	Yes
Total cholesterol in HDL3	q20metab_HDL3_C	Yes
Esterified cholesterol	q20metab_EstC	Yes
Free cholesterol	q20metab_FreeC	Yes
Serum total triglycerides	q20metab_Serum_TG	Yes
Triglycerides in VLDL	q20metab_VLDL_TG	Yes
Triglycerides in LDL	q20metab_LDL_TG	Yes
Triglycerides in HDL	q20metab_HDL_TG	Yes
Diacylglycerol	q20metab_DAG	Yes
Ratio of diacylglycerol to triglycerides	q20metab_DAG_TG_ratio	Yes
Total phosphoglycerides	q20metab_TotPG	Yes
Ratio of triglycerides to phosphoglycerides	q20metab_TG_PG_ratio	Yes
Phosphatidylcholine and other cholines	q20metab_PC	Yes
Sphingomyelins	q20metab_SM	Yes
Total cholines	q20metab_TotCho	Yes
Apolipoprotein A-I	q20metab_ApoA1	Yes
Apolipoprotein B	q20metab_ApoB	Yes
Ratio of apolipoprotein B to apolipoprotein A-I	q20metab_ApoB_ApoA1_ratio	Yes
Total fatty acids	q20metab_TotFA	Yes
Estimated description of fatty acid chain length, not actual carbon number	q20metab_FALen	Yes
Estimated degree of unsaturation	q20metab_UnSat	Yes
22:6, docosahexaenoic acid	q20metab_DHA	Yes

18:2, linoleic acid	q20metab_LA	Yes
Conjugated linoleic acid	q20metab_CLA	Yes
Omega-3 fatty acids	q20metab_FAw3	Yes
Omega-6 fatty acids	q20metab_FAw6	Yes
Polyunsaturated fatty acids	q20metab_PUFA	Yes
Monounsaturated fatty acids, 16:1,18:1	q20metab_MUFA	Yes
Saturated fatty acids	q20metab_SFA	Yes
Ratio of 22:6 docosahexaenoic acid to total fatty acids	q20metab_DHA_FA_ratio	Yes
Ratio of 18:2 linoleic acid to total fatty acids	q20metab_LA_FA_ratio	Yes
Ratio of conjugated linoleic acid to total fatty acids	q20metab_CLA_FA_ratio	Yes
Ratio of omega-3 fatty acids to total fatty acids	q20metab_FAw3_FA_ratio	Yes
Ratio of omega-6 fatty acids to total fatty acids	q20metab_FAw6_FA_ratio	Yes
Ratio of polyunsaturated fatty acids to total fatty acids	q20metab_PUFA_FA_ratio	Yes
Ratio of monounsaturated fatty acids to total fatty acids	q20metab_MUFA_FA_ratio	Yes
Ratio of saturated fatty acids to total fatty acids	q20metab_SFA_FA_ratio	Yes
Glucose	q20metab_Glc	Yes
Lactate	q20metab_Lac	Yes
Pyruvate	q20metab_Pyr	Yes
Citrate	q20metab_Cit	Yes
Glycerol	q20metab_Glcl	Yes
Alanine	q20metab_Ala	Yes
Glutamine	q20metab_Gln	Yes
Glycine	q20metab_Gly	Yes
Histidine	q20metab_His	Yes
Isoleucine	q20metab_Ile	Yes
Leucine	q20metab_Leu	Yes
Valine	q20metab_Val	Yes
Phenylalanine	q20metab_Phe	Yes
Tyrosine	q20metab_Tyr	Yes
Acetate	q20metab_Ace	Yes
Acetoacetate	q20metab_AcAce	Yes
3-hydroxybutyrate	q20metab_bOHBut	Yes
Creatinine	q20metab_Crea	Yes
Albumin	q20metab_Alb	Yes
Glycoprotein acetyls, mainly a1-acid glycoprotein	q20metab_Gp	Yes