

SUPPLEMENTARY MATERIAL

Spousal associations of serum metabolomic profiles by nuclear magnetic resonance spectroscopy

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Table S1: NMR metabolic measures

Molecular class	Lipid, lipoprotein or metabolite name	Units*
Extremely large VLDL	Concentration of chylomicrons and extremely large VLDL particles	mol/l
	Total lipids in chylomicrons and extremely large VLDL	mmol/l
	Phospholipids in chylomicrons and extremely large VLDL	mmol/l
	Total cholesterol in chylomicrons and extremely large VLDL	mmol/l
	Free cholesterol in chylomicrons and extremely large VLDL	mmol/l
	Triglycerides in chylomicrons and extremely large VLDL	mmol/l
Very large VLDL	Concentration of very large VLDL particles	mol/l
	Total lipids in very large VLDL	mmol/l
	Phospholipids in very large VLDL	mmol/l
	Total cholesterol in very large VLDL	mmol/l
	Cholesterol esters in very large VLDL	mmol/l
	Free cholesterol in very large VLDL	mmol/l
	Triglycerides in very large VLDL	mmol/l
Large VLDL	Concentration of large VLDL particles	mol/l
	Total lipids in large VLDL	mmol/l
	Phospholipids in large VLDL	mmol/l
	Total cholesterol in large VLDL	mmol/l
	Cholesterol esters in large VLDL	mmol/l
	Free cholesterol in large VLDL	mmol/l
	Triglycerides in large VLDL	mmol/l
Medium VLDL	Concentration of large VLDL particles	mol/l
	Total lipids in small VLDL	mmol/l
	Phospholipids in small VLDL	mmol/l
	Total cholesterol in small VLDL	mmol/l
	Cholesterol esters in small VLDL	mmol/l
	Free cholesterol in small VLDL	mmol/l
	Triglycerides in small VLDL	mmol/l
Small VLDL	Concentration of very small VLDL particles	mol/l
	Total lipids in very small VLDL	mmol/l
	Phospholipids in very small VLDL	mmol/l
	Total cholesterol in very small VLDL	mmol/l
	Cholesterol esters in very small VLDL	mmol/l
	Free cholesterol in very small VLDL	mmol/l
	Triglycerides in very small VLDL	mmol/l
IDL	Concentration of IDL particles	mol/l
	Total lipids in IDL	mmol/l
	Phospholipids in IDL	mmol/l
	Total cholesterol in IDL	mmol/l
	Cholesterol esters in IDL	mmol/l
	Free cholesterol in IDL	mmol/l
	Triglycerides in IDL	mmol/l
Large LDL	Concentration of large LDL particles	mol/l

	Total lipids in large LDL	mmol/l
	Phospholipids in large LDL	mmol/l
	Total cholesterol in large LDL	mmol/l
	Cholesterol esters in large LDL	mmol/l
	Free cholesterol in large LDL	mmol/l
	Triglycerides in large LDL	mmol/l
Medium LDL	Concentration of medium LDL particles	mol/l
	Total lipids in medium LDL	mmol/l
	Phospholipids in medium LDL	mmol/l
	Total cholesterol in medium LDL	mmol/l
	Cholesterol esters in medium LDL	mmol/l
	Free cholesterol in medium LDL	mmol/l
	Triglycerides in medium LDL	mmol/l
Small LDL	Concentration of small LDL particles	mol/l
	Total lipids in small LDL	mmol/l
	Phospholipids in small LDL	mmol/l
	Total cholesterol in small LDL	mmol/l
	Cholesterol esters in small LDL	mmol/l
	Free cholesterol in small LDL	mmol/l
	Triglycerides in small LDL	mmol/l
Very large HDL	Concentration of very large HDL particles	mol/l
	Total lipids in very large HDL	mmol/l
	Phospholipids in very large HDL	mmol/l
	Total cholesterol in very large HDL	mmol/l
	Cholesterol esters in very large HDL	mmol/l
	Free cholesterol in very large HDL	mmol/l
	Triglycerides in very large HDL	mmol/l
Large HDL	Concentration of large HDL particles	mol/l
	Total lipids in large HDL	mmol/l
	Phospholipids in large HDL	mmol/l
	Total cholesterol in large HDL	mmol/l
	Cholesterol esters in large HDL	mmol/l
	Free cholesterol in large HDL	mmol/l
	Triglycerides in large HDL	mmol/l
Medium HDL	Concentration of medium HDL particles	mol/l
	Total lipids in medium HDL	mmol/l
	Phospholipids in medium HDL	mmol/l
	Total cholesterol in medium HDL	mmol/l
	Cholesterol esters in medium HDL	mmol/l
	Free cholesterol in medium HDL	mmol/l
	Triglycerides in medium HDL	mmol/l
Small HDL	Concentration of small HDL particles	mol/l
	Total lipids in small HDL	mmol/l
	Phospholipids in small HDL	mmol/l
	Total cholesterol in small HDL	mmol/l
	Cholesterol esters in small HDL	mmol/l
	Free cholesterol in small HDL	mmol/l

	Triglycerides in small HDL	mmol/l
Lipoprotein particle size	Mean diameter for VLDL particles	nm
	Mean diameter for LDL particles	nm
	Mean diameter for HDL particles	nm
Cholesterol concentrations	Total cholesterol	mmol/l
	Total cholesterol in VLDL	mmol/l
	Remnant cholesterol (non-HDL and non-LDL cholesterol)	mmol/l
	Total cholesterol in LDL	mmol/l
	Total cholesterol in HDL	mmol/l
	Total cholesterol in HDL2	mmol/l
	Total cholesterol in HDL3	mmol/l
	Esterified cholesterol	mmol/l
	Free cholesterol	mmol/l
Glycerides and phospholipid concentrations (and one ratio)	Total triglycerides	mmol/l
	Triglycerides in VLDL	mmol/l
	Triglycerides in LDL	mmol/l
	Triglycerides in HDL	mmol/l
	Total phosphoglycerides	mmol/l
	Ratio of triglycerides to phosphoglycerides	
	Phosphatidylcholine and other cholines	mmol/l
	Sphingomyelins	mmol/l
	Total cholines	mmol/l
Apolipoprotein concentrations (and one ratio)	Apolipoprotein A-1	g/l
	Apolipoprotein B	g/l
Fatty acid concentrations	Total fatty acids	mmol/l
	Estimated degree of saturation	
	22:6, docosaheptaenoic acid	mmol/l
	18:2 linoleic acid	mmol/l
	Omega-3 fatty acids	mmol/l
	Omega-6 fatty acids	mmol/l
	Polyunsaturated fatty acids	mmol/l
	Monounsaturated fatty acids; 16:1, 18:1	mmol/l
	Saturated fatty acids	mmol/l
Fatty acid ratios	Ratio of 22:6, docosaheptaenoic acid to total fatty acids	%
	Ratio of 18:2 linoleic acid to total fatty acids	%
	Ratio of omega-3 fatty acids to total fatty acids	%
	Ratio of omega-6 fatty acids to total fatty acids	%
	Ratio of polyunsaturated fatty acids to total fatty acids	%
	Ratio of monounsaturated fatty acids to total fatty acids	%
	Ratio of saturated fatty acids to total fatty acids	%
Glycolysis related metabolite	Glucose	mmol/l
	Lactate	mmol/l
	Pyruvate	mmol/l
	Citrate	mmol/l
	Glycerol	mmol/l
	Alanine	mmol/l

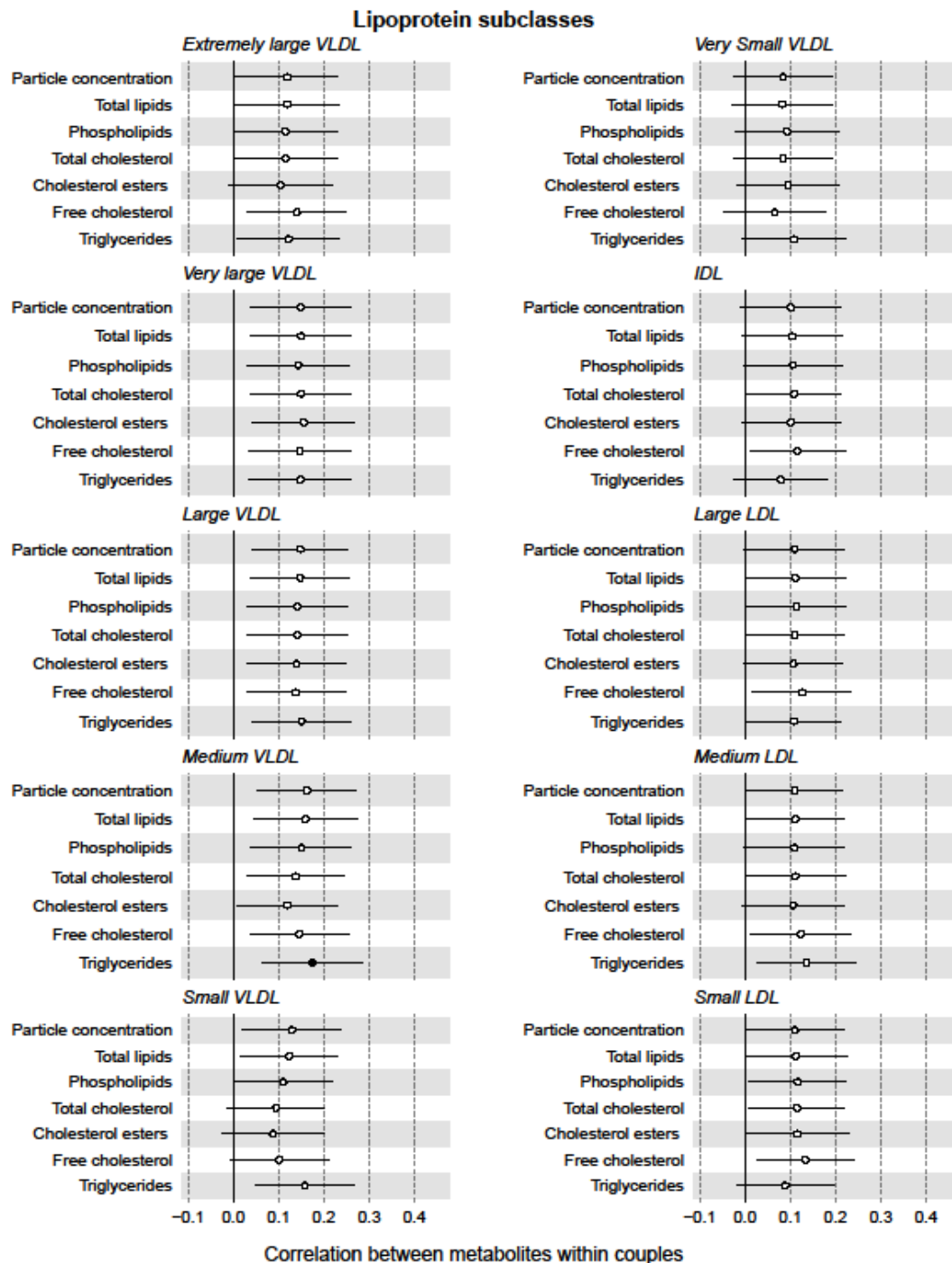
	Glutamine	mmol/l
Amino acid concentrations	Glycine	mmol/l
	Histidine	mmol/l
branched	Isoleucine	mmol/l
branched	Leucine	mmol/l
branched	Valine	mmol/l
aromatic	Phenylalanine	mmol/l
aromatic	Tyrosine	mmol/l
Ketone body concentrations	Acetate	mmol/l
	Acetoacetate	mmol/l
	3-hydroxybutyrate	mmol/l
Fluid balance marker	Albumin	mmol/l
	Creatinine	mmol/l
Inflammation marker	Glycoprotein acetyls, mainly a1-acid glycoprotein	mmol/l

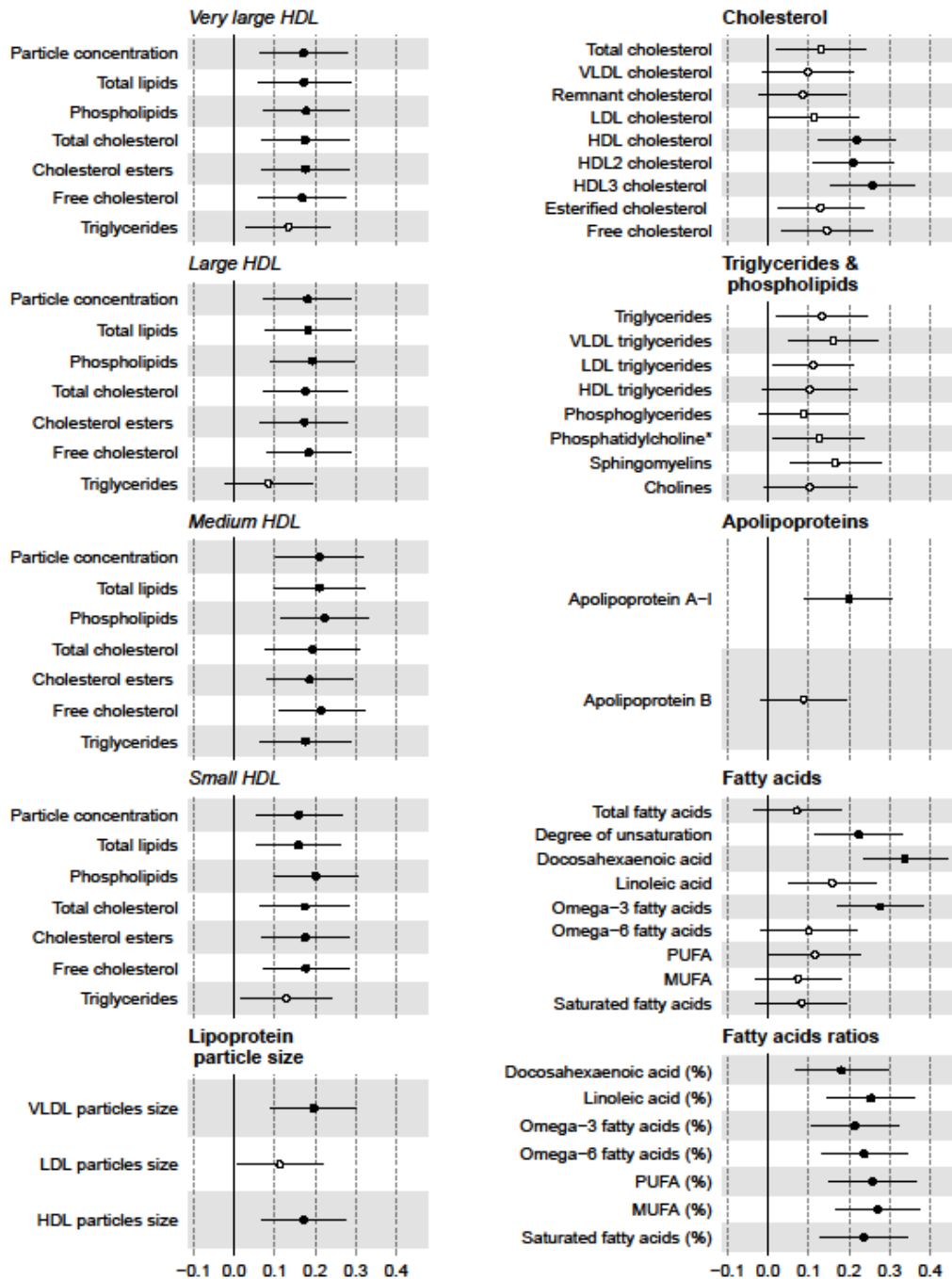
* These are the units used throughout the paper for each of the metabolic measures, unless we state that we are presenting results in standard deviation (SD) units. Where we present results that are the mean (in control participants) at 16-weeks these are the units. Where we present change in metabolic marker (between 16- to 36-weeks) or difference in change of metabolic markers the units are those listed in the table above per one week of gestational age.

VLDL: very low density lipoprotein; LDL: low density lipoprotein; IDL: intermediate density lipoprotein; HDL: high density lipoprotein

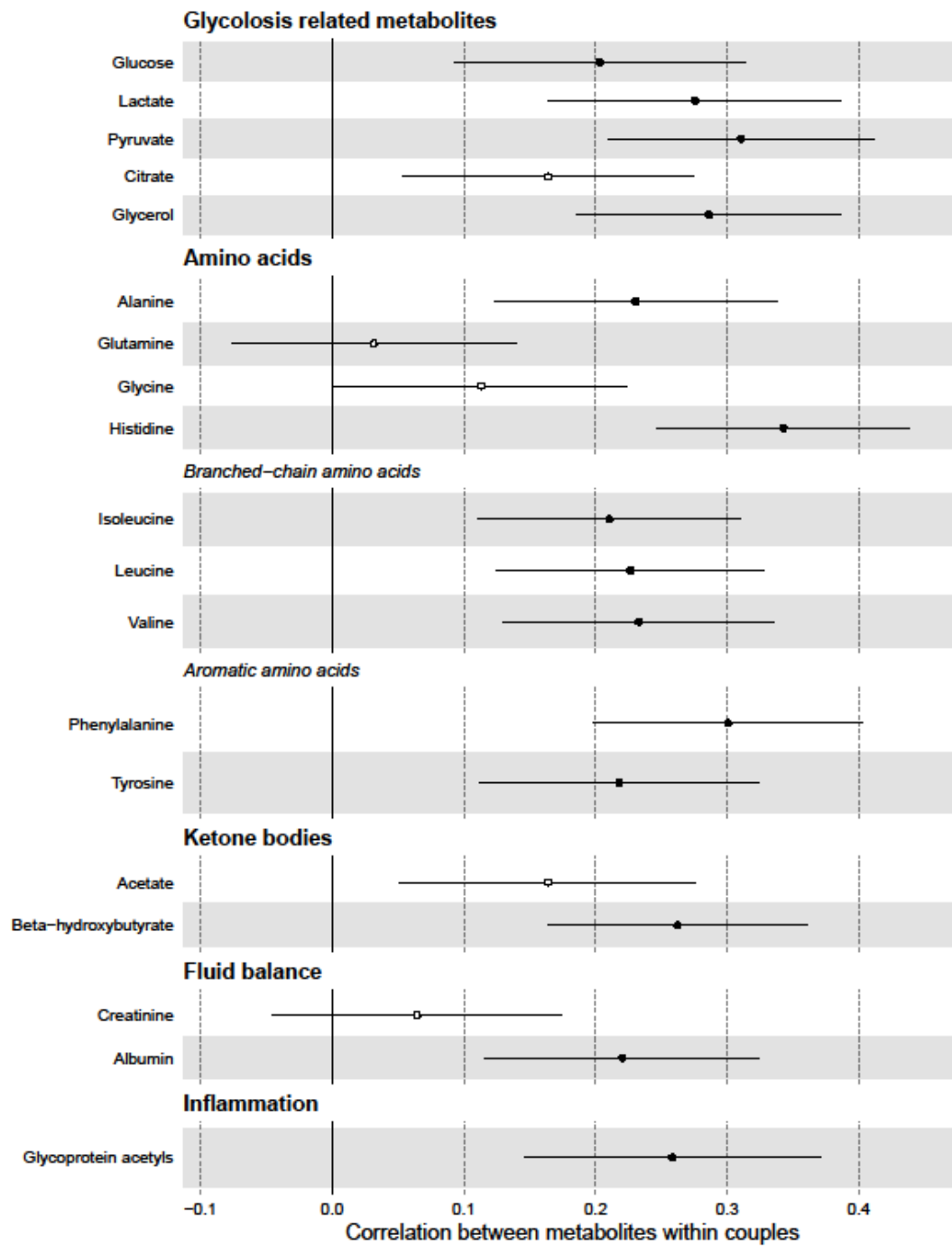
Supplementary Figures

Supplemental Figure S1. Spearman correlations of metabolic measures in couples awaiting IVF.



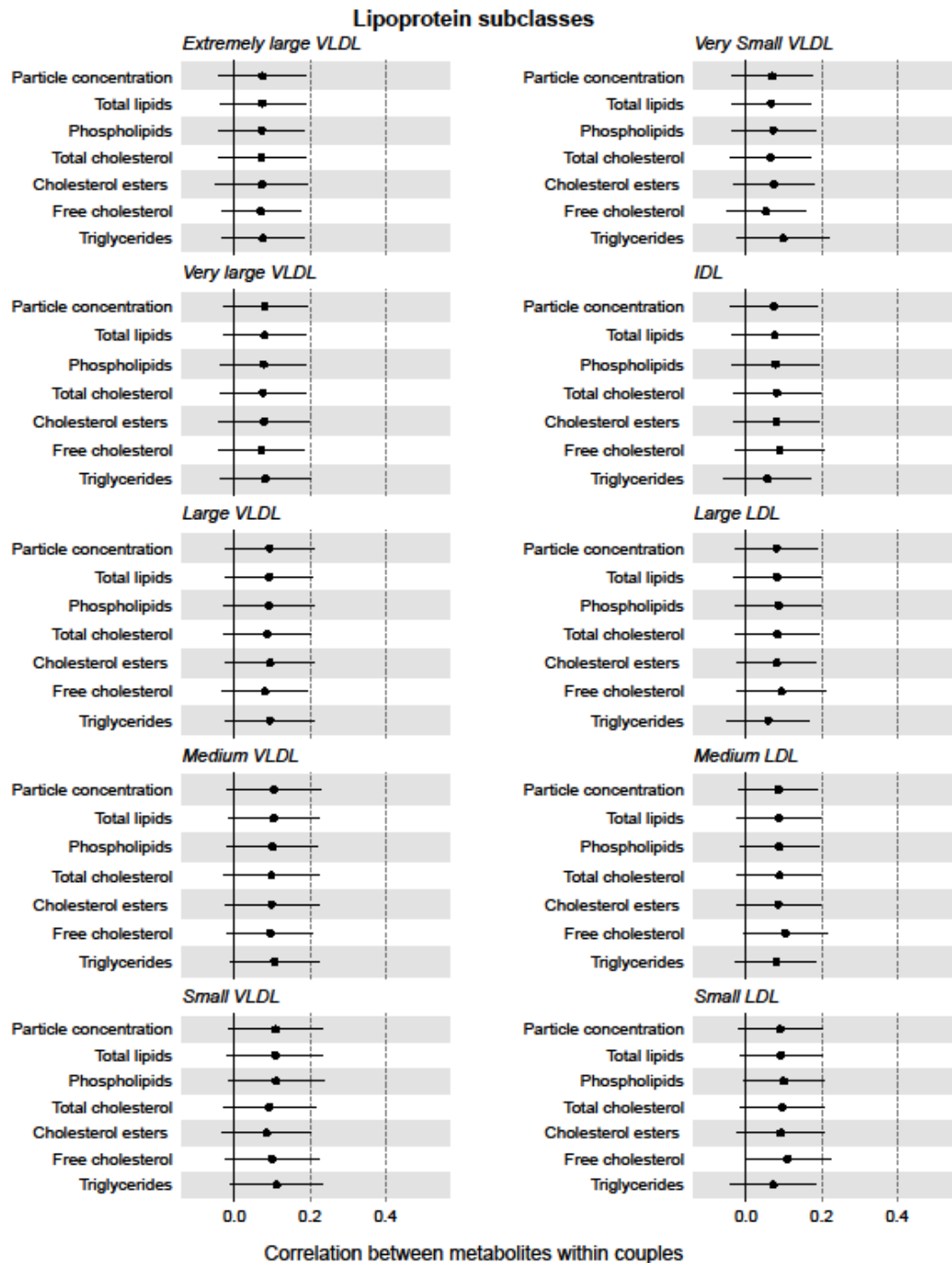


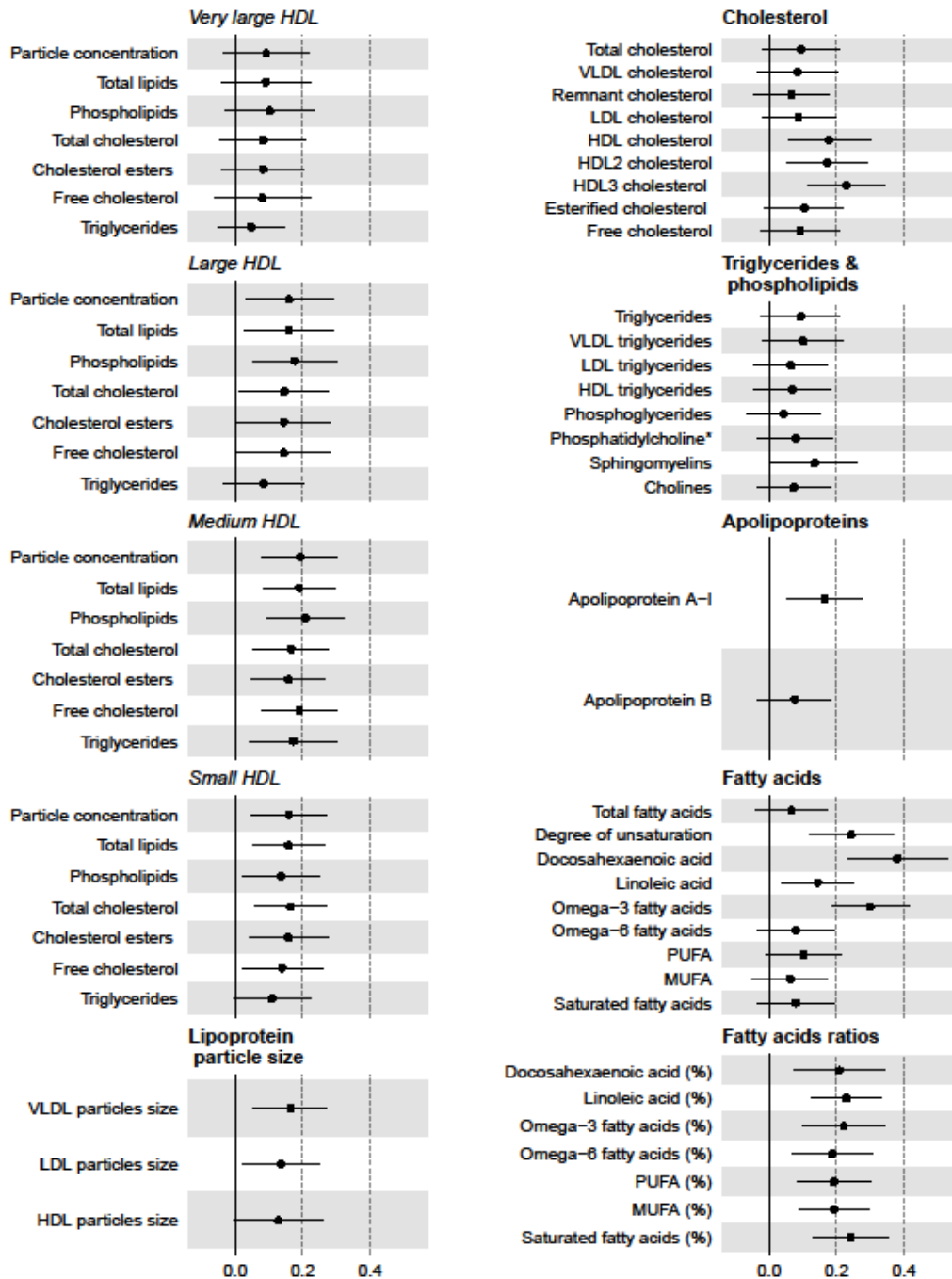
Correlation between metabolites within couples



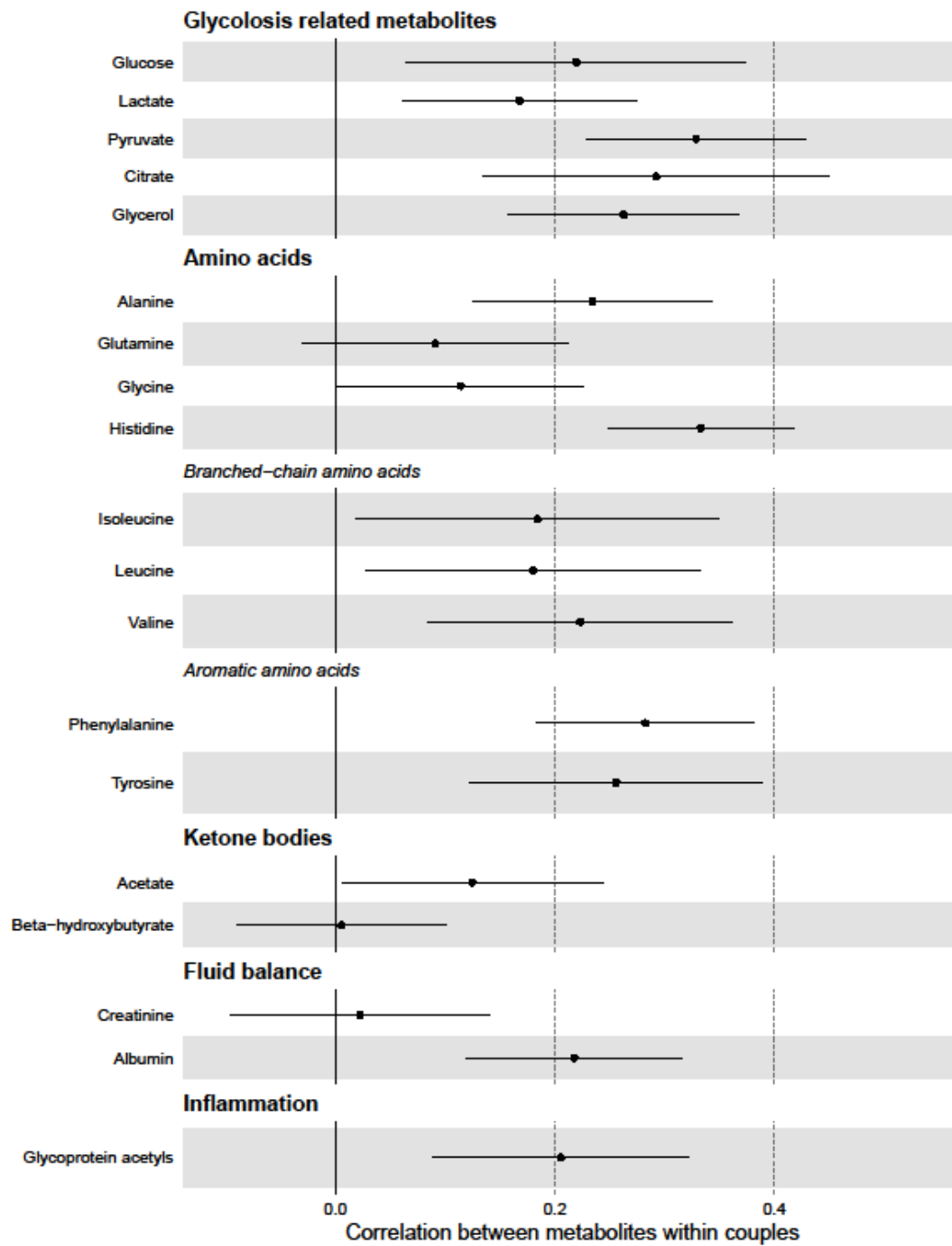
Supplemental Figure S2. Adjusted correlations of metabolic measures in couples awaiting IVF.

Pearson correlation coefficients and 95%CI of male and female linear regression residuals after sex-specific adjustment for age, educational attainment, ever smoking, physical activity, family history of cardiometabolic disease, alcohol consumption, BMI, and ethnicity.



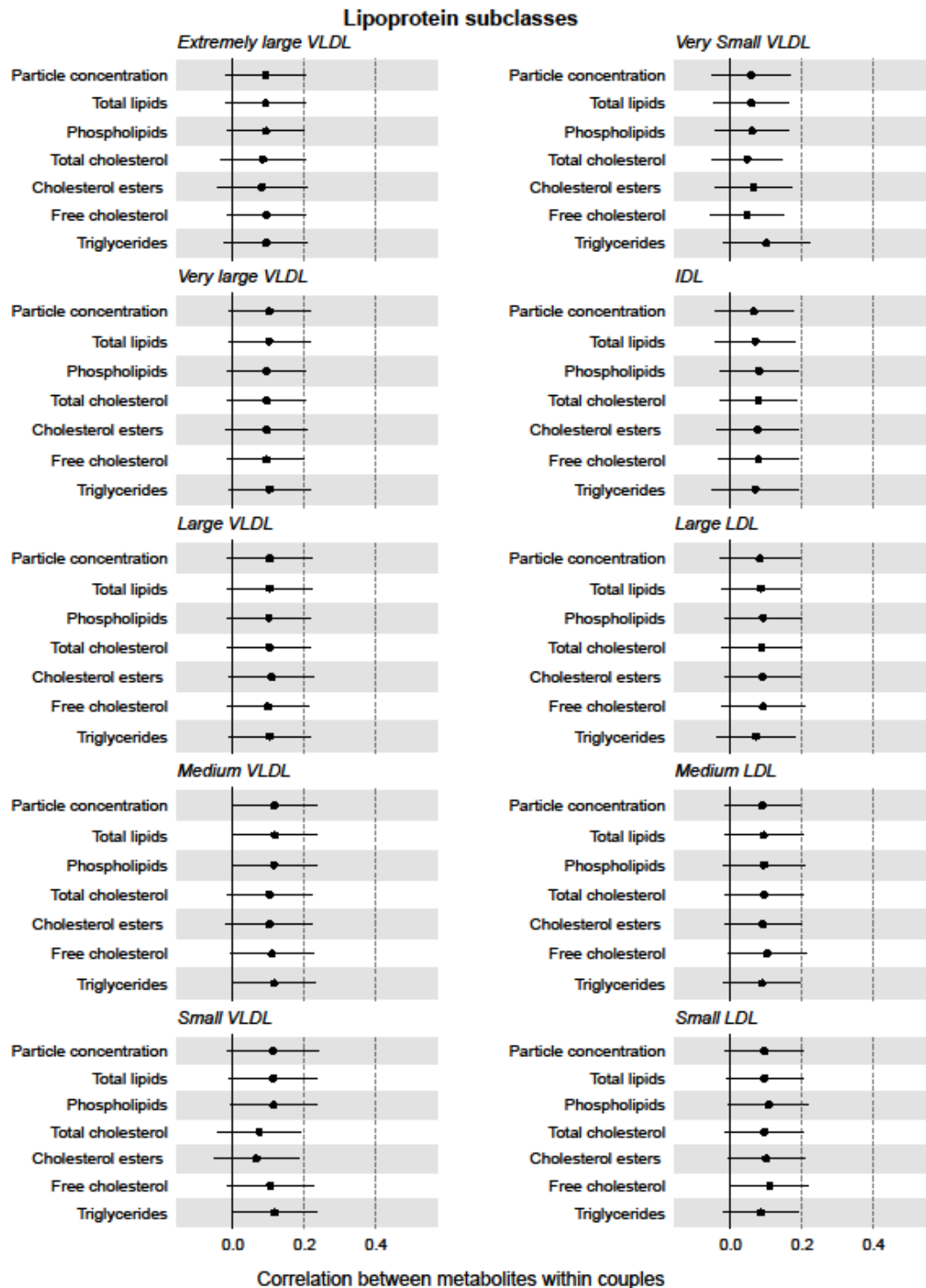


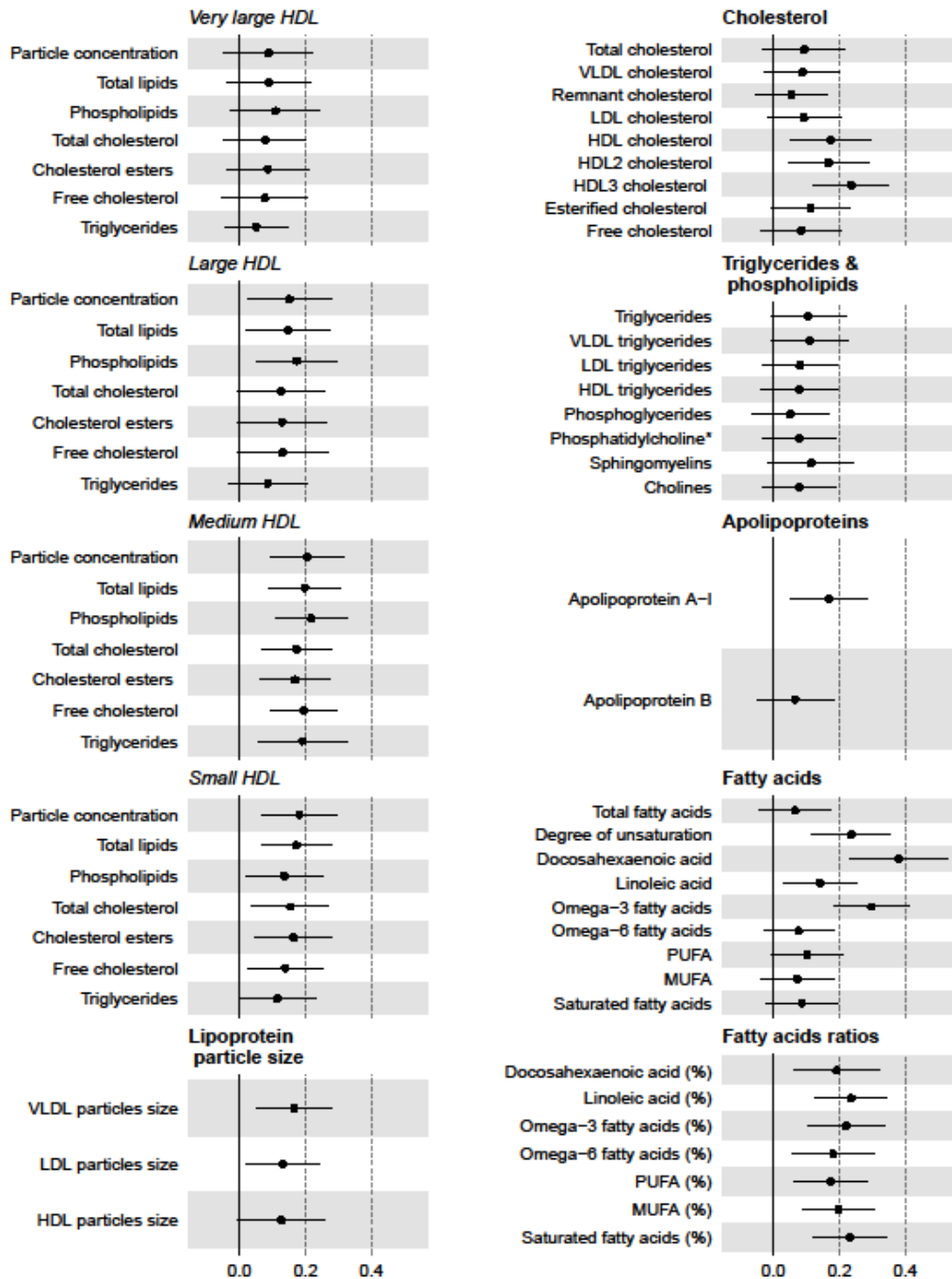
Correlation between metabolites within couples



Supplemental Figure S3. Correlations of metabolic measures in couples awaiting IVF using quantile regression.

Pearson correlation coefficients and 95%CI of male and female quantile regression residuals after sex-specific adjustment for age, educational attainment, ever smoking, physical activity, family history of cardiometabolic disease, alcohol consumption, BMI, and ethnicity.





Correlation between metabolites within couples

