File S5 Volcano plots of VO2peak-associated plasma metabolite patterns
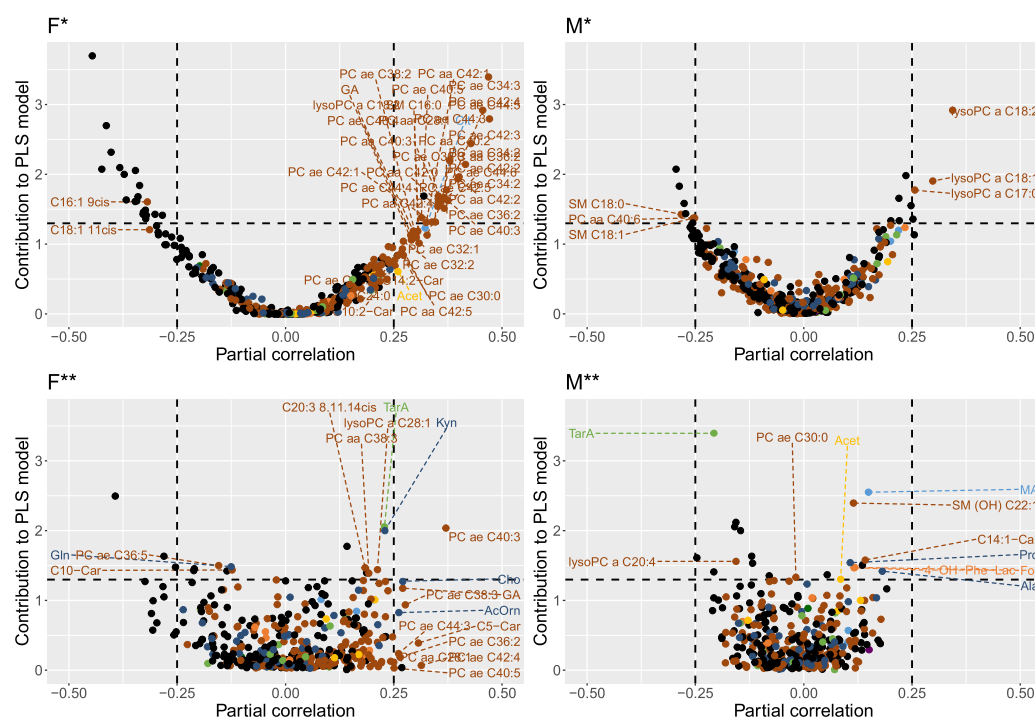
F*   Females adjusted for age and menopausal status
F**   Females adjusted for age, menopausal status and the 21 phenotypical and clinical parameters
M*   Males adjusted for age
M**   Males adjusted for age and the 21 phenotypical and clinical parameters

Major Metabolic Pathways:

        Lipid metabolism   Amino acid metabolism   Xenobiotics and related metabolism
        Energy metabolism   Carbohydrate metabolism   Mammalian-microbial cometabolism
        Nucleotide metabolism   Cofactors and vitamins metabolism   Unknown

Volcano plots illustrating sex-specific plasma metabolite patterns associated with the VO2peak for each subgroup. The y-axis represents the importance of contribution of each metabolite to the multivariate association with the VO2peak, expressed as the negative logarithm of relative frequencies of permutation-obtained rank products below measured rank products. The x-axis illustrates the direction and strength of bivariate associations between the VO2peak and metabolites, expressed as partial Pearson correlation coefficients of Van der Waerden-transformed variables. The classification of metabolites to major metabolic pathways is color-coded. The mean of the root mean square error (RMSE) based on the test samples was not always higher in the permutations when additionally controlling for phenotypical and clinical variables. Therefore, the respective results from multivariate association analyses (F**/M**) have to be interpreted with caution.