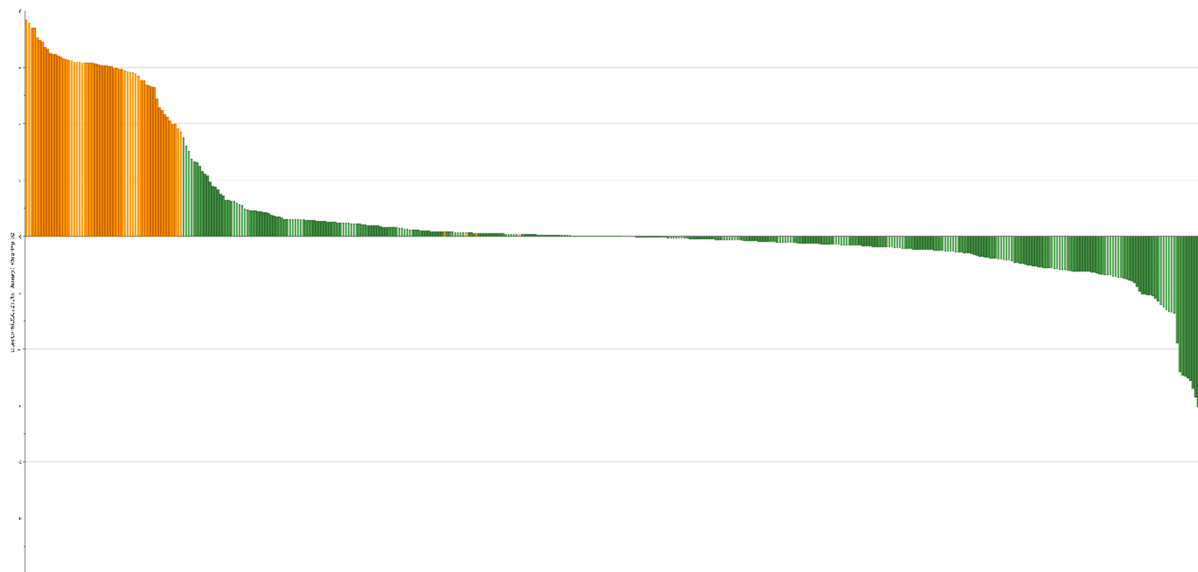


Supplementary Materials S1



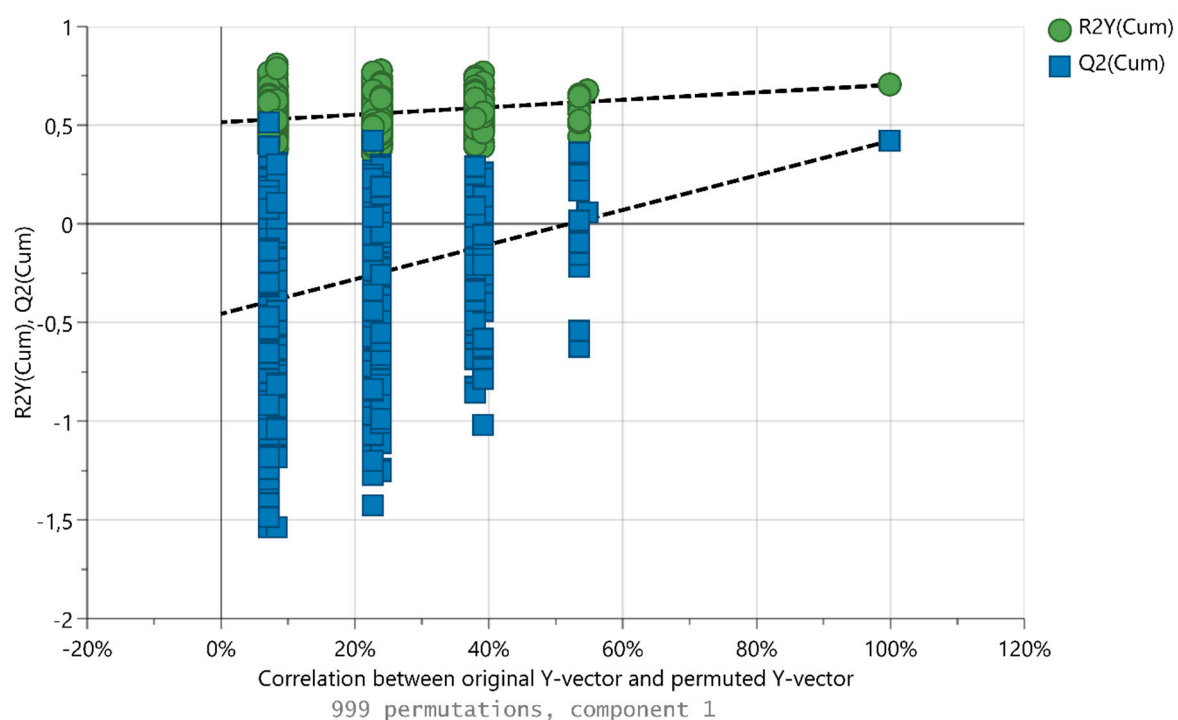
Above is a **contribution plot for patient Zic015**. Each column represents a X-variable, i.e., each column expresses the score contribution (called Weight) of each variable expressed as the difference between the individual in question and the average. Coloring is by SIMCA-default, orange columns showing the variables that contribute the most for Zic015. Below, for purposes of interpretation, we list the most important (“orange”) variables, in falling order of Weight. Note that glc=glucose and that the suffix C denotes cerebrospinal fluid:

Name of X-variable	Weight
beta-glc (attenuated) 67 C	7.65321
glc+gln 211 C	7.58669
493 C	7.03222
beta-glc (attenuated) 68 C	6.90862
glc 285 C	6.73999
491 C	6.6743
492 C	6.66529
glc 217 C	6.63557
glc 276 C	6.55021
alpha-glc 56 C	6.43098
glc+fructose 173 C	6.42943
alpha-glc 57 C	6.33893
glc 277 C	6.31861
298 C	6.27931
glc+fructose 176 C	6.20533
glc 275 C	6.20264
glc 274 C	6.19837
glc 194 C	6.17351
glc+fructose 174 C	6.16794
glc 219 C	6.15058

glc+fructose 177 C	6.1368
glc 278 C	6.09901
glc 271 C	6.0944
glc 196 C	6.08112
glc 189 C	6.06117
glc 218 C	6.04696
glc 190 C	6.03791
glc 309 C	6.00169
glc 199 C	5.98645
glc 200 C	5.98247
glc+fructose 222 C	5.94988
glc 216 C	5.94664
glc 307 C	5.92836
glc 215 C	5.90836
glc 269 C	5.87302
glc 310 C	5.85255
glc 272 C	5.85083
glc 273 C	5.85083

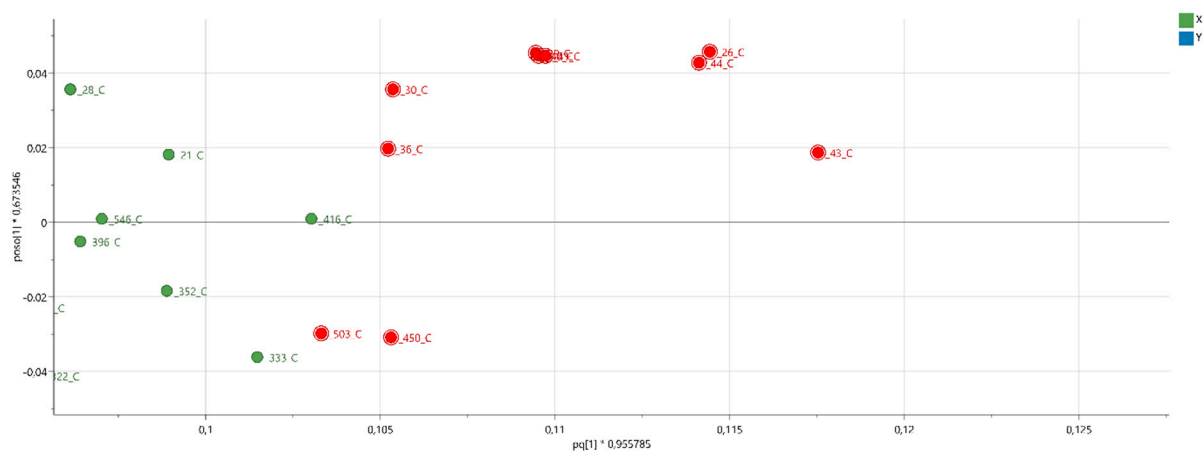
Hence, almost all important variable in the contribution plot are associated with glucose.

Supplementary Materials S2



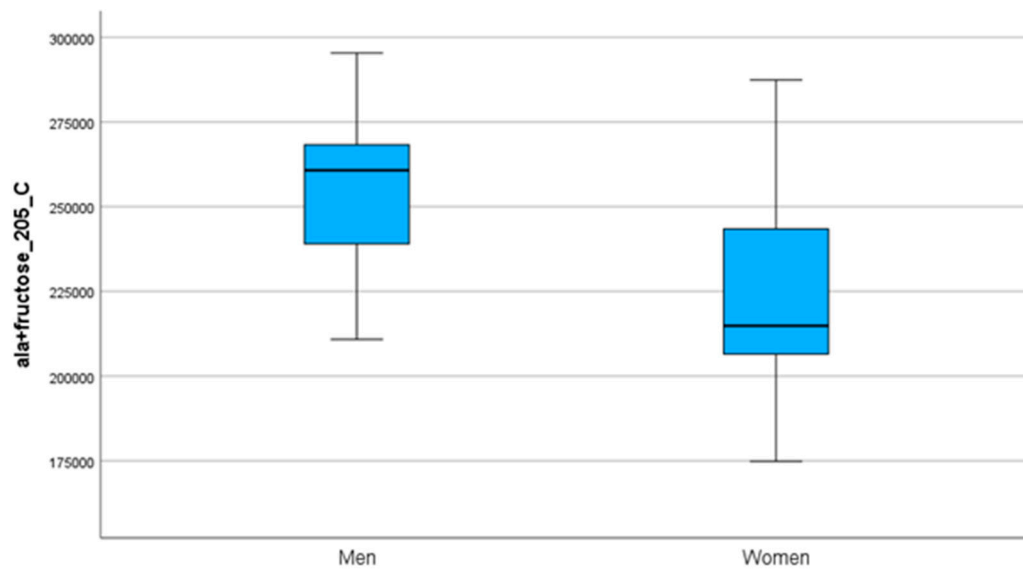
This is a permutation plot which confirms the validity of the OPLS-DA model, the intercept for Q2 being <0.

Supplementary Materials S3



This is a zoomed-in part of the loading plot of the OPLS-DA model of patients vs. healthy controls. In other words, this is a part of the loading plot corresponding to the score plot depicted in **Figure 1** in the main text. The features mentioned in the paper are in red. Note especially the extremely high inter-correlation of 29_C, 40_C and 41_C; so much so that the three are almost merged in the plot. This is confirmed by the fact that the corresponding bivariate correlation coefficients for these three features range 0.981-0.995 (Spearman's rho, see **Table 3** in the main text).

Supplementary Materials S4



This box plot illustrates feature “ala+fructose_205_C” in patients, comparing men and women ($p=0.125$).