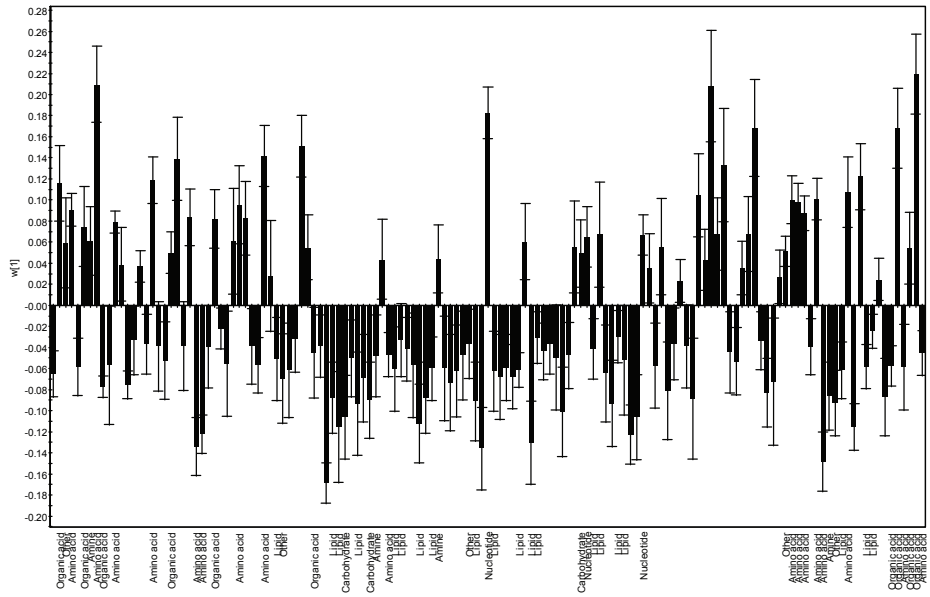

Figure 2_supplementary. Predictive loadings (w) for the significant metabolites between "Low CO_2" and "High CO_2" samples, at 3h (see Fig. 4 for overview of all detected metabolites). Significantly differing metabolites were detected by interpreting the first weight vector (w[1]), as described by (Trygg and Wold, 2002), from the OPLS-DA model described in figure 4, together with the 95% confidence intervals calculated using jack-knifing (Martens and Martens, 2000). . Positive values indicate higher concentrations for "Low CO_2" samples and negative values indicate higher concentrations for "High CO_2" samples. Metabolites are named after compound class. Metabolites not classified are unknown metabolites not possible to classify.

References:

Martens H, Martens M (2000) Modified Jack-knife estimation of parameter uncertainty in bilinear modelling by partial least squares regression (PLSR). Food Qual Pref **11:** 5-16

Trygg J, Wold S (2002) Orthogonal projections to latent structures (OPLS). J Chemometrics **16:** 119-128