Figure S1

Box-plots showing the distribution of the coefficients of variation of 417 lipids in QC samples from the data for the sample sets of short-term (A) and long-term (B) analysis, respectively . "Short term" means exposure of whole blood from 27 individuals for 0.5h, 1h and 1.5 h to either 4°C, or 21°C or 30°C. "Long term" means exposure of whole blood from 56 individuals for 2h, 4h and 24h to either 4°C, or 21°C or 30°C.
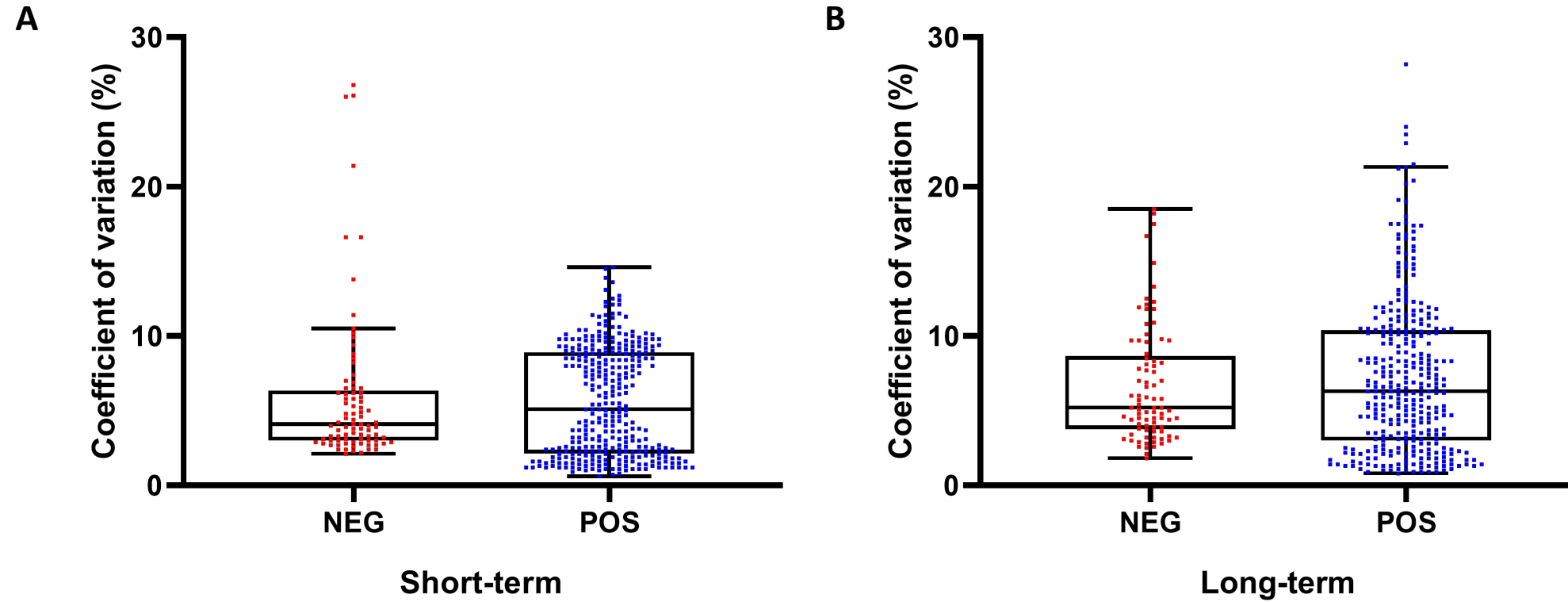
Figure S2.

Scheme of the workflow for the identification of a lipid pattern as a possible tool to assess the sample quality.

Elucidation of a lipid pattern out of 417 lipids to identify samples of questionable quality

Step 1: stringent sample quality definition (perfect vs worst)

0h	30°C 24h
Good	Bad

Linear regression (149 lipids) — 114 lipids — Unstable lipids (129 lipids)

Lasso regression for feature selection

6 lipids

Step 2: extensive quality definition for samples

Stepwise logistic regression

	0.5h	1h	1.5h	2h	4h	24h
4°C	Good	Good	Good	Good	Good	Bad
21°C	Good	Bad	Bad	Bad	Bad	Bad
30°C	Bad	Bad	Bad	Bad	Bad	Bad

LPC 16:1
LPE 20:4 } Lipid panel
LPC O-18:1

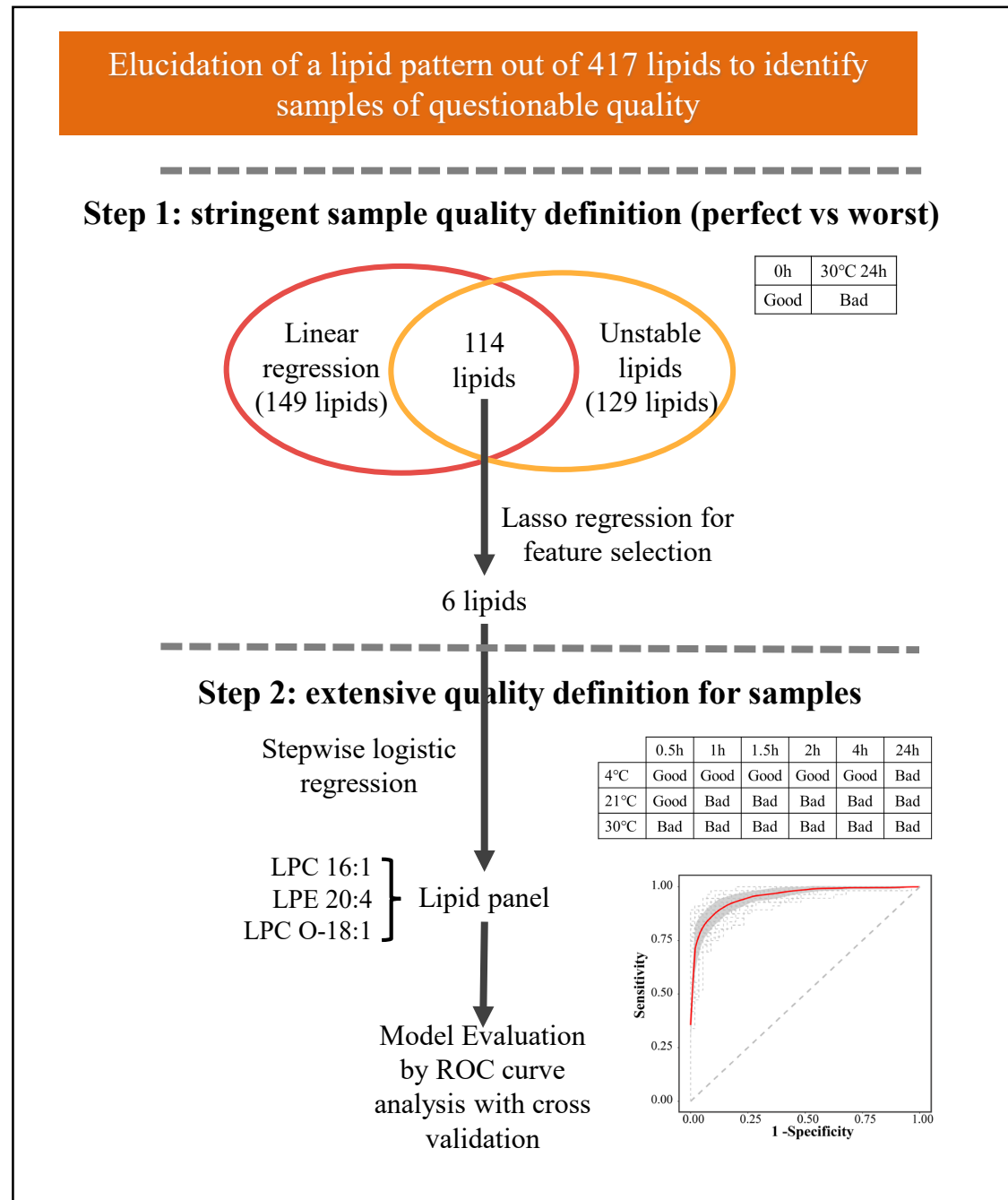Model Evaluation by ROC curve analysis with cross validation

Figure S3.
Area under the receiver operating characteristic (ROC) curve (AUC) of the lipid triplet panel based on 10 times repeated 5-fold cross validation.