Supplementary material

Towards Fatty Acid Determination in Human Milk by Attenuated Total Reflection Infrared Spectroscopy and Solvent-Free Lipid Separation

Christopher K. Akhgar [1], Vanessa Nürnberger [2], Marlene Nadvornik [1], Victoria Ramos-Garcia [3], Isabel Ten-Doménech [3], Julia Kuligowski [3], Andreas Schwaighofer [1], Erwin Rosenberg [1] and Bernhard Lendl [1,*]

[1] Institute of Chemical Technologies and Analytics, Technische Universität Wien, Getreidemarkt 9, 1060 Vienna, Austria

[2] Competence Center CHASE GmbH, Altenberger Straße 69, 4040 Linz, Austria

[3] Neonatal Research Group, Health Research Institute La Fe, Avda Fernando Abri Martorell 106, 46026 Valencia, Spain

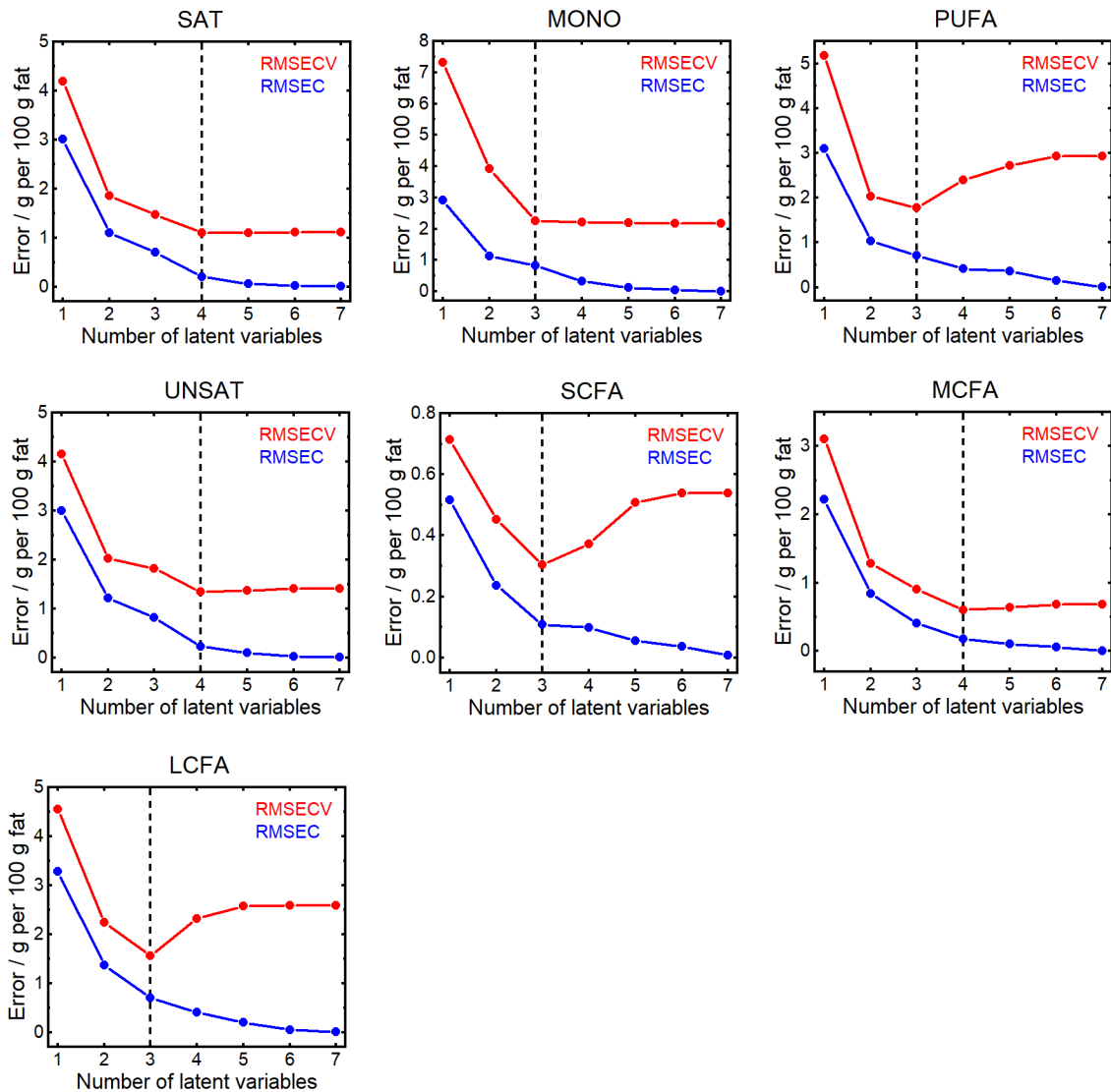* Correspondence: bernhard.lendl@tuwien.ac.at; Tel.: +43/1/58801-15140

Figure S1. Root mean square error of cross validation (RMSECV, red) and root mean square error of calibration (RMSEC, blue), depending on the number of latent variables. The dashed lines indicate the selected number of latent variables for each individual PLS model. SAT: saturated fatty acids; MONO: monounsaturated fatty acids; PUFA: polyunsaturated fatty acids; UNSAT: unsaturated fatty acids; SCFA: short-chain fatty acids (C4–C10); MCFA: medium-chain fatty acids (C12–C16); LCFA: long-chain fatty acids (C17 and higher).
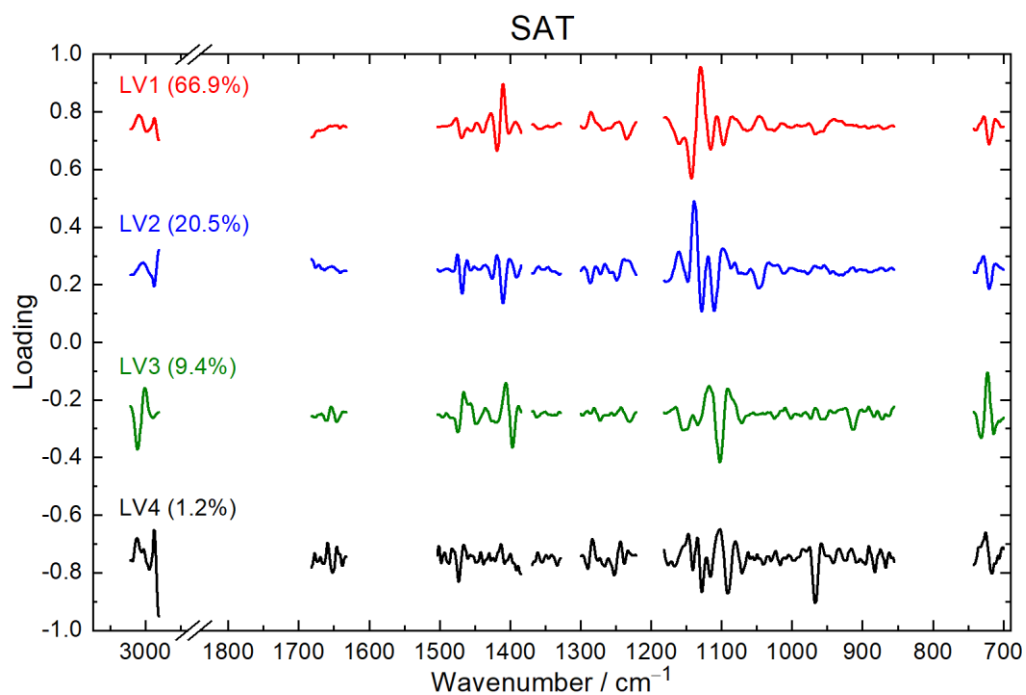
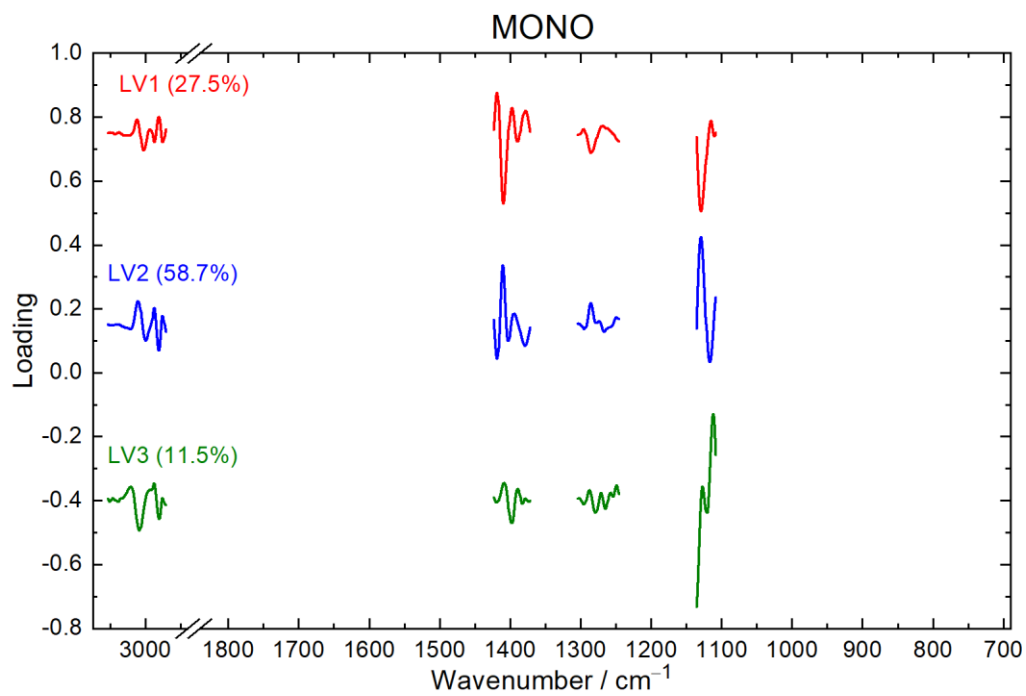**Figure S2.** Loading plot of saturated fatty acids.

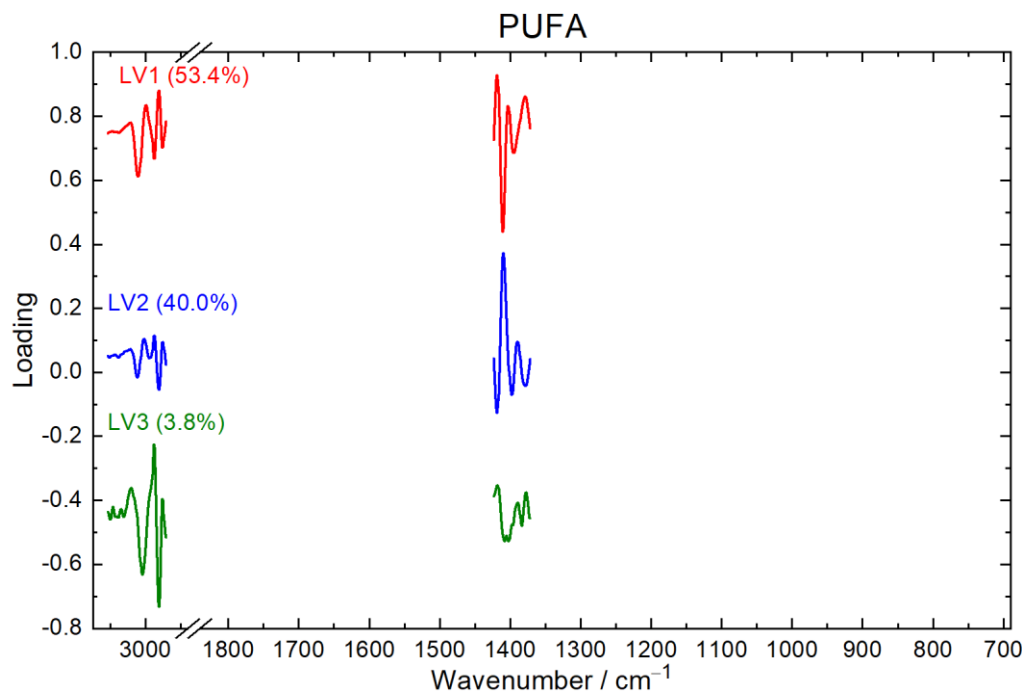**Figure S3.** Loading plot of monounsaturated fatty acids.

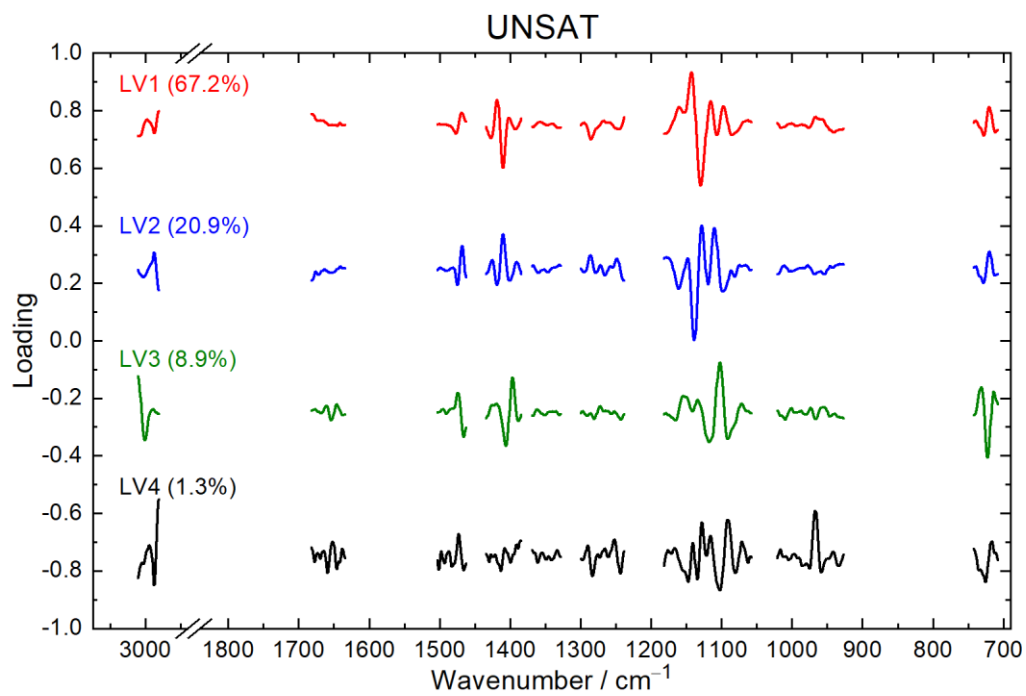**Figure S4.** Loading plot of polyunsaturated fatty acids.
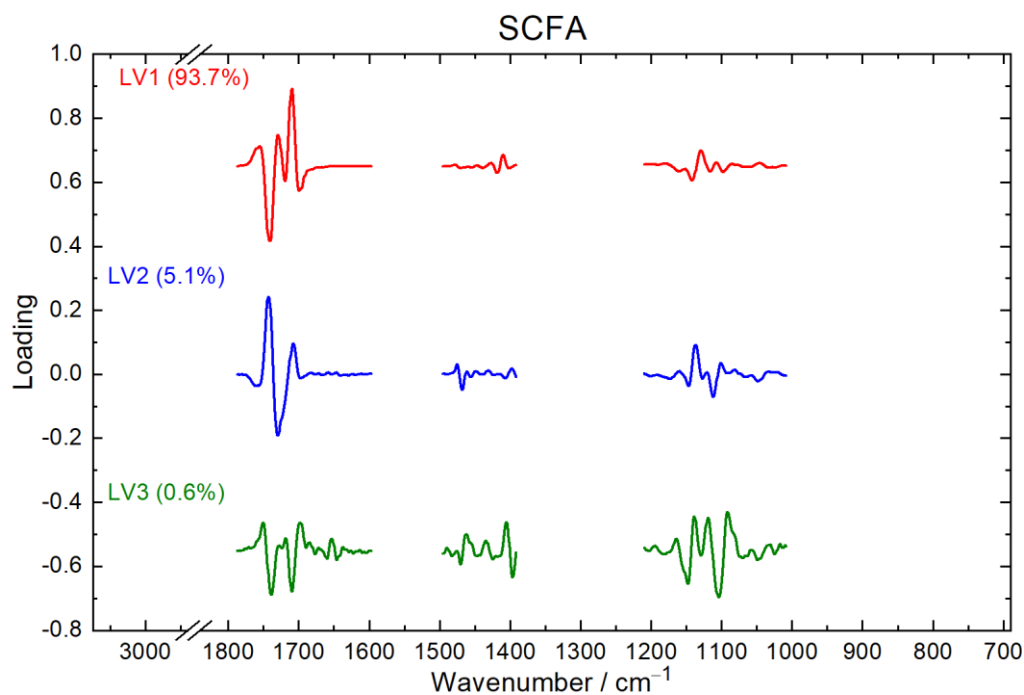

Figure S5. Loading plot of unsaturated fatty acids.
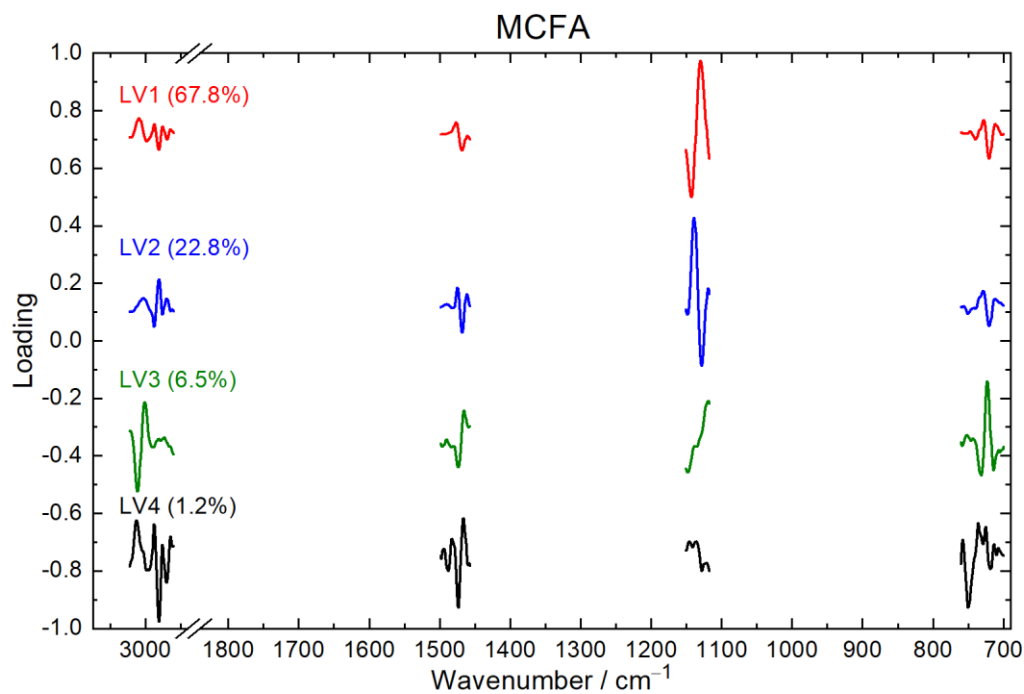
Figure S6. Loading plot of short-chain fatty acids.
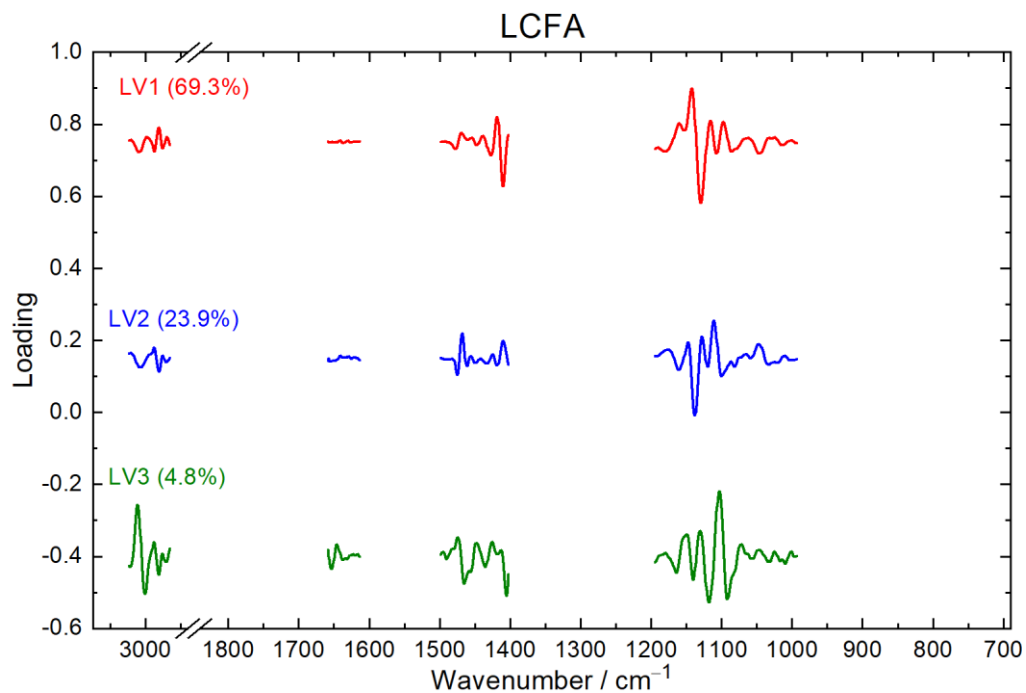

Figure S7. Loading plot of medium-chain fatty acids.

Figure S8. Loading plot of long-chain fatty acids.