NMR-Based Metabolomics of the Lipid Fraction of Organic and Conventional Bovine Milk

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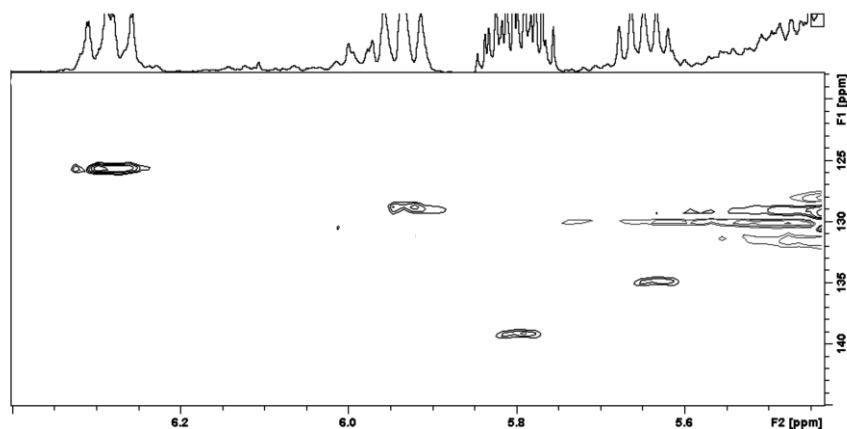
Figure S1. Selected region of 500 MHz ^{1}H-^{13}C HSQC spectrum of the lipid fraction of a lyophilized bovine milk sample in CDCl[3] illustrating [1]H-^{13}C connectivities of conjugated (9-*cis*,11-*trans*)18:2 linoleic acid (CLA) and caproleic acid; T, 298 K; 40 repetitions of 256 increments, total experimental time 4 h 35 min.
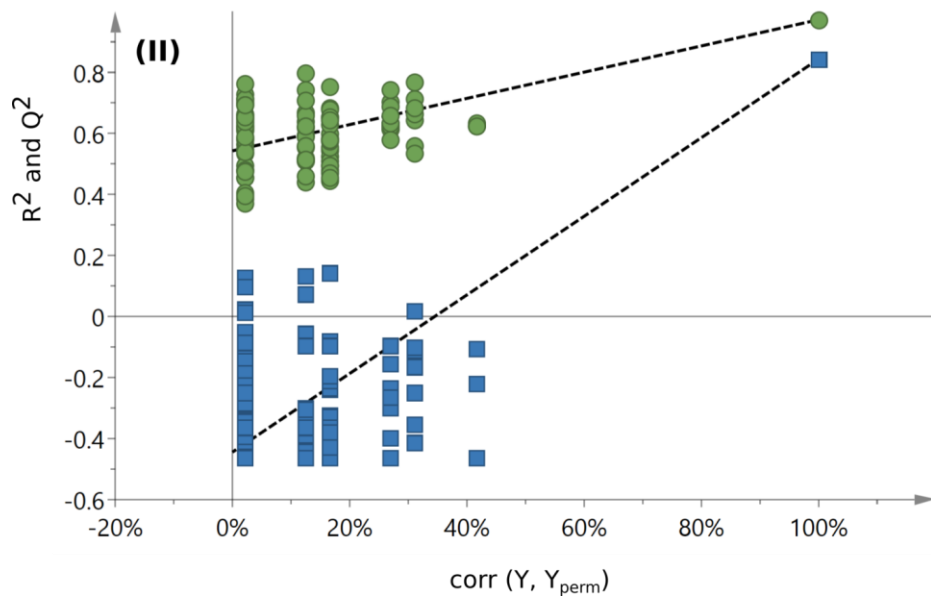
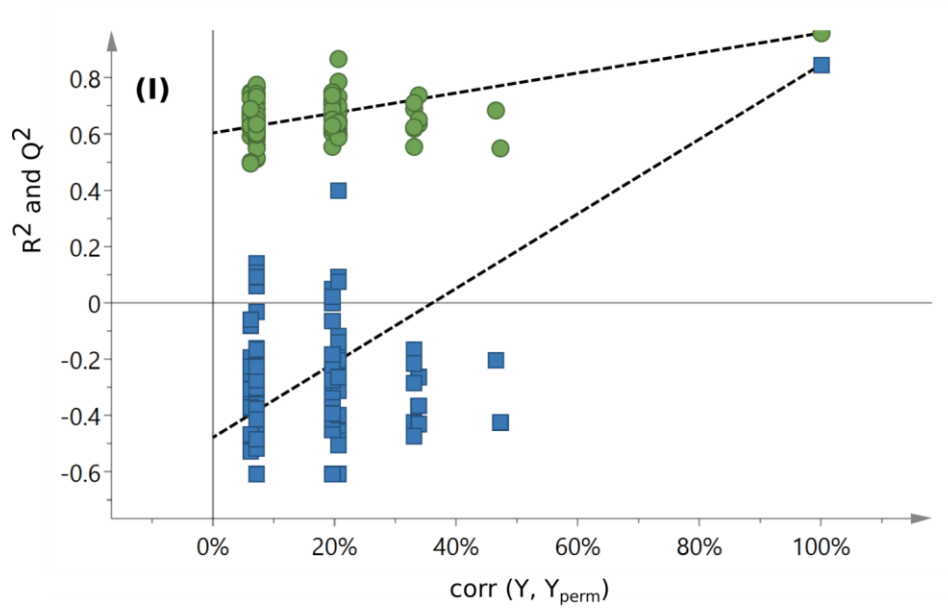**Figure S2.** Permutation test of the P samples with PLS-DA: **(I)** UNor method, **(II)** NorCont method.
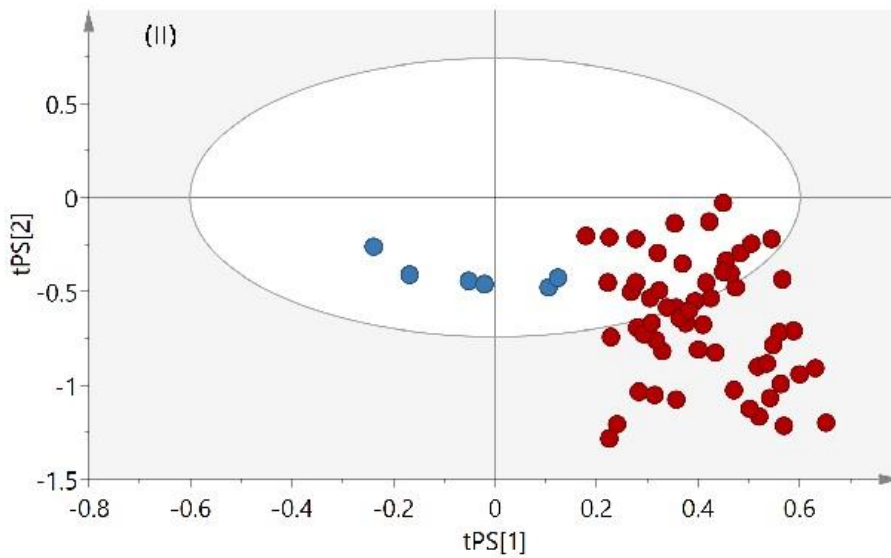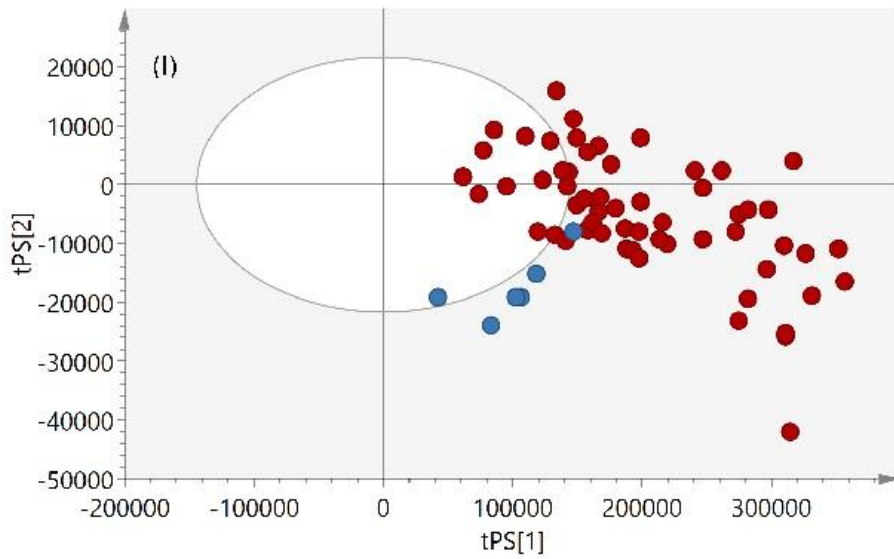
Figure S3. Predicted Score Plot of the R samples (as test set) using P samples as a prediction set: (**I**) UNor method, (**II**) NorCont method (blue circles: organic milk samples, red circles: conventional milk samples).

(b)

(a)

100
80
60
40
20
0

Relative Amplitude (%)

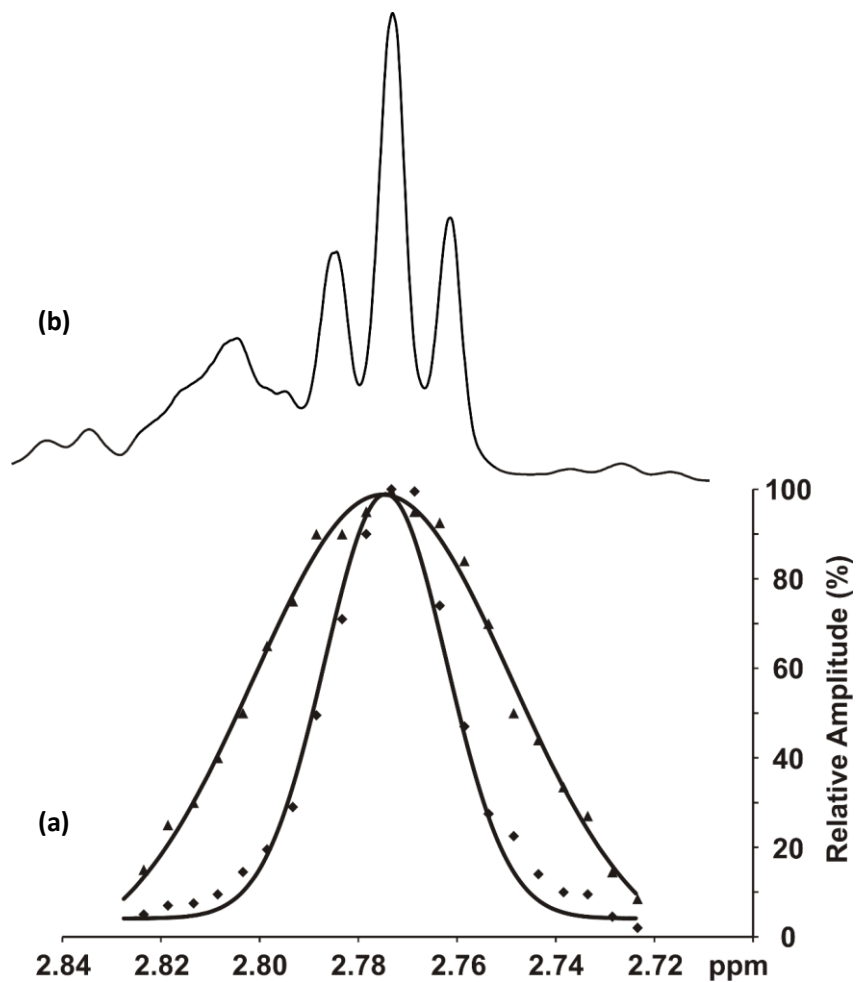2.84   2.82   2.80   2.78   2.76   2.74   2.72   ppm

Figure S4. (**a**) Selectivity of the excitation bandwidth of the shaped pulse of 20 ms (▲) and 80 ms (♦) of the 1D TOCSY experiment. The carrier frequency of the shaped pulse was set in both cases at δ = 2.77 ppm. (**b**) For comparison the apparent triplets of the allylic protons of linoleic acid (δ = 2.77 ppm) and α-linolenic acid (δ = 2.81 ppm) of the 1D ^{1}H NMR spectrum of the lipid fraction of ~~lyoplilized~~ lyophilized bovine milk sample in CDCl$_3$ are presented.
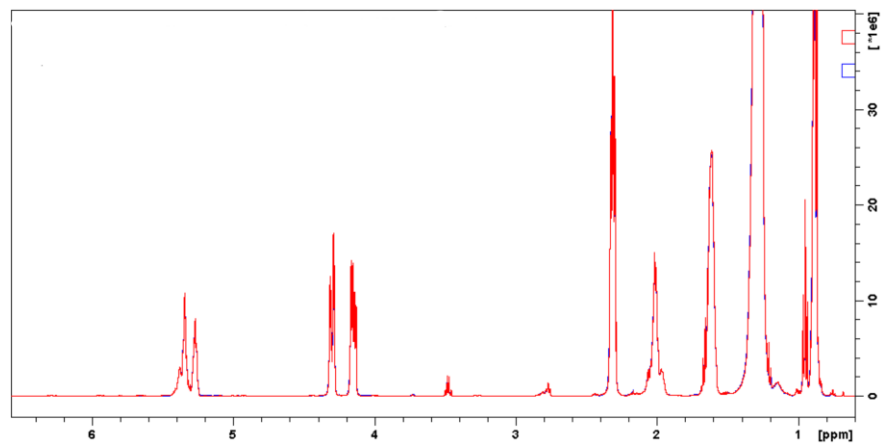
Figure S5. 500 MHz ¹H NMR spectra of the lipid fraction of a lyophilized bovine milk sample in CDCl₃; T, 298 K; ~~Number~~ number of scans, 256 ; recycle time, 9.3 s̶.̶ (blue color) and 14.5 s (red color).