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# Verification of the identity of fats and oils

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## Abstract

Verification of the identity of fats and oils remains a challenge. This paper presents a fingerprint approach, which is illustrated by comparison of butter fat and two of its fractions. Regular butter fat and its soft and hard fractions were analysed for their fatty acid (FA) and triacylglycerol compositions using gas chromatography (GC). The identities of the product groups were predicted by applying Partial Least Square Discriminant Analysis (PLS-DA) with ten-fold cross-validation. The classification based on the FA dataset and TAG dataset resulted in 91% and 82% success rates, respectively.

## Materials and Methods

Eight regular and fourteen fractionated butter fat samples (8 soft and 6 hard fractions) were kindly provided by VIV Vreeland (Zelhem, NL) and Friesland Foods (Noordwijk, NL). The FA compositions were determined by methylation of the fats and analysis of the FA methyl esters according to ISO15885:2002. Nonanoic acid was added as internal standard. The TAG analysis was carried out according to Draft International Standard ISO/DIS 17678 | IDF202. Tricaprion (C18) was added as internal standard and the reference material CRM 519 (IRMM, Geel, B) was used for determining the calibration factor of each triglyceride. All samples were analysed in triplicate. PLS:DA models were estimated to predict the identity of the samples using either the FA or TAG data (Matlab: PLS toolbox). Model performance was evaluated by means of 10:fold cross: validation. Standardization on variables and units, as well as the number of components was varied to optimize prediction rates.

## Results and Discussion

The FA and TAG compositions of the butter fats were determined. The compositions were characterized by 18 FAs and 17 TAGs. After optimization of the data standardization and model component numbers, hundred cross-validations were run to gain insight into the stability of the results. For FA, one hard fraction was consistently classified as soft, and one soft fraction samples as regular butter fat. The results of one particular cross validation run are listed in Table 1. A scores plot of the two dimensions of the model is presented in Fig. 1. Two samples (FA analysis) were misclassified.

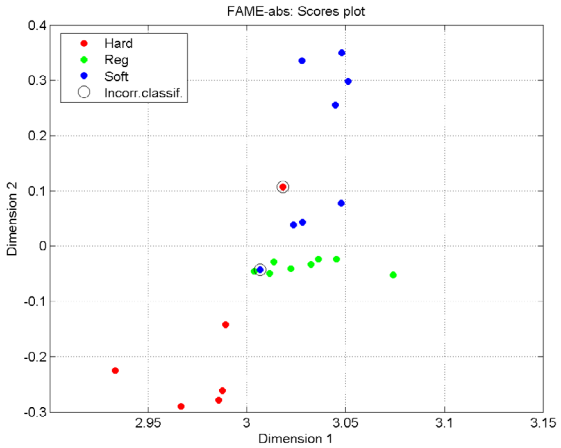


*Fig. 1. Scores plot of the first two dimensions of PLS:DA on the fatty acid compositional data of regular and fractionated butter fats.*

*Table 1. PLS-DA classification rates of regular and fractionated butter oils by their FA and TAG compositions using two component PLS-DA models: correctly classified in bold**

| | PLS-DA classification | | | | | |
|---|---|---|---|---|---|---|
| | FA | | | TAG | | |
| | Hard | Reg | Soft | Hard | Reg | Soft |
| Hard fraction | **83%** | 0% | 17% | **50%** | 17% | 33% |
| Regular fat | 0% | **100%** | 0% | 0% | **88%** | 13% |
| Soft fraction | 0% | 13% | **87%** | 0% | 0% | **100%** |

**Different superscripts in a row indicate significant differences (P<0.05).*

The scores plot reveals that these samples are positioned in the middle of the classes they were allocated to. The results of one cross validation run for the TAG data (Table 1) show that three hard fraction samples were misclassified, two as soft fraction samples and one as a regular butter fat. It is remarkable that one of the samples was also misclassified when their FA data were used. Their PLS-DA plot (not shown) shows that one of the hard fraction samples is in the middle of the soft fraction samples. The others are close to the demarcation line.

## Conclusions

The present study shows a promising multivariate approach for verification of the identity of fats and fat fractions: on average prediction was successful for 91% (FA) and 82% (TAG) of the samples.

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