## RESEARCH ARTICLE

Mass Spectrometry



## Design of a Prediction Model for the Differentiation of Pasteurized Milk from Heated ESL Milk by Peptide Profiling

Sevim Dalabasmaz and Monika Pischetsrieder\*

This study designs a prediction model to differentiate pasteurized milk from heated extended shelf life (ESL) milk based on milk peptides. For this purpose, quantitative peptide profiles of a training set of commercial samples including pasteurized (n = 20), pasteurized-ESL (n = 13), and heated-ESL (n = 13) = 16) milk are recorded by matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF-MS). Seven peptides are selected as putative markers, and cutoff levels and performance measures of each marker are defined by receiver operating characteristic (ROC) analysis. The accuracy of these peptides in the training set range between 71% and 90%. A prediction model is established based on the combined cutoff levels and evaluated by an independent blind test set. The processing method of 19 out of 20 unknown milk samples is predicted correctly achieving 95% accuracy. Five peptides of the prediction model are identified as  $\alpha_{S1}$ -casein<sub>182-199</sub> (m/z 2014.0),  $\alpha_{S1}$ -casein<sub>180-199</sub> (m/z 2216.1),  $\alpha_{S1}$ -casein<sub>1-24</sub> (m/z 2910.6),  $\beta$ -casein<sub>108-125</sub> (m/z 2126.0), and  $\beta$ -casein<sub>106-125</sub> (m/z 2391.2)indicating thermal release and the action of plasmin and cathepsins. Thus, the present study demonstrates that the milk peptide profile reflects even minor differences in production parameters.