## Abstract

One of the most relevant group of toxicologically significant compounds in beer are N-nitrosamines. In this thesis, the attention was paid especially on non-volatile nitroso compounds whose concentrations in beer, a chemical structure, and a biological effect has not been known yet. For the reason of the lack of knowledge regarding this compound group, the method for their sensitive detection by chemiluminescence detection after gas chromatographic separation was developed. This method permits a classification of detected nitroso compounds to different groups (N-nitroso, C-nitroso, and combination of C-nitroso and nitro) and distinguish them from interferences. The method is based on recording of a pyrolytic profile of each chromatographic peak, the profiles are then processed by discriminant analysis. The method has been developed for finding and structural identification purposes of these unknown compounds. Its application on an artificially nitrosated beer sample, together with gas chromatographic tandem mass spectrometric analysis, led to structural identification of several representatives of nitroso compounds.

Sensory active compounds in this thesis are represented by carbonyl compounds and fatty acids. Carbonyl compounds – furfural and hydroxymethylfurfural – were used during the development of mobile, easy-to-use, rapid, and objective *in situ* method for stale flavor intensity of beer determination – stale flavor is a reflection of inappropriate storage condition of beer. The method is based on color reaction on the test strip, reflectometric detection, and the calibration model performed by data from sensory and chemical analysis of a real samples. Resulted method permits determination of stale flavor of beer on four-point scale, with uncertainty ± 0.5 and limit of determination 1.0.

The last experimental part of this thesis is focused on study of distribution of fatty acids during the brewing process by analytical-chemometric tool named sensomic profiling. Some of the new patterns of fatty acid formation during the brewing process was uncovered.