

Abstract

This dissertation thesis summarizes results of experiments that have been carried out during my PhD studies related to the new mass spectrometric methods for trace gas analysis of human breath.

The thesis is divided into the theoretical and experimental part. The chapter at the beginning of this dissertation summarizes the current research in the area of breath analysis. It is describing the common breath metabolites, benefits and challenges of the method for therapeutic monitoring and clinical diagnosis and current applications. The next chapter of the theoretical introduction describes the techniques suitable for this area of research, with a special emphasis on mass-spectrometric techniques (in particular the selected ion flow tube mass spectrometry, SIFT-MS, method that allows accurate quantification of trace gases and vapours in humid air/human breath). All these parts are elaborated via the scientific literature review.

The following chapters are then directly related to my own research and describes the conducted experiment, including the results obtained. This experimental part “Results and Discussion” is divided to the individual subsections, which are conceived as the commentaries to the enclosed research papers published in peer reviewed journals. The first is the detailed step by step overview of the kinetics of ion molecule reactions (the basis of SIFT-MS) including the determination of rate constants and product branching ratios for several ion-molecule reactions of H_3O^+ , NO^+ and O_2^+ reagent ions with carboxylic acids and possible Inflammatory Bowel Disease, IBD, biomarkers. The latter subsections are focused on three-body association reactions related to experiments, where the samples are influenced by the presence of water vapour (case of breath analysis), and on optimization of SIFT-MS kinetic library for accurate quantifications by this method. The last two sections finally concern the application of SIFT-MS for the breath analysis and describe not only results gathered in the area of IBD, but also challenges, which are connected with the off-line analysis and utilisation of Nalophan sampling bags, that have been encountered during my research - mainly the problematic of impurities released from the Nalophan sampling bags (off line analysis), that could significantly involve the SIFT-MS breath analysis, where low-level substances are determined.