Abstract

This thesis describes research that has been carried out during the years 2009-2013 as a part of my PhD project related to the method of selected ion flow tube mass spectrometry (SIFT-MS) and its application in interdisciplinary areas of research. SIFT-MS is a method that allows accurate quantification of trace gases and vapours presented in humid air with the focus on human breath; without any sample preparation and in real time.
The thesis is divided into several parts. The first part reviews the history of mass spectrometry as a background for the quantitative analytical methods as PTR-MS and SIFT-MS. The second part discusses the detailed history of development of SIFT-MS, starting from principles of selected ion flow tube (SIFT) technique that has been used for study of ion-molecule reactions in the gas phase and forms the basis of SIFT-MS. The next part discusses volatile organic compounds of different biological origin: bacterial, plant and human breath metabolites that can be analyzed in real time using SIFT-MS.
The main part "Results and Discussion" is divided into several subsections that serve as commentaries to the enclosed research papers published in peer reviewed journals. The first is a detailed step by step overview of the kinetics of ion molecule reactions which is the basis of SIFT-MS including the determination of rate constants and product branching ratio for several ion-molecule reactions of H_3O^+, NO^+ and $O_2^{+\bullet}$ precursor ions with six phytogenic esters and seven isomers of hexanol. Other two sections concern the application of SIFT-MS in the discovery of biomarkers for clinical diagnostic of inflammatory bowel disease and infections complicating cystic fibrosis. Next section covers a study of population dynamics of three different bacterial species based on their volatile signatures. The theme of plant physiology and the volatiles that are released by plants in the process of phytovolatilization is discussed in the following section. The final section discusses an application of SIFT-MS in the field of security research for the study of decomposition of a highly energetic explosive FOX-7.