Letter

Comparison of pyridine and pyrazine derivatives distribution in exhaled breath and exhaled breath condensate after smoking

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Molecular mass distributions of series of compounds found in exhaled breath after smoking are compared between the direct-breath analysis by extractive electrospray ionization and the analysis of exhaled breath condensate by direct-infusion electrospray ionization mass spectrometry. Although all the analyzed series of compounds are detected by both methods, their relative abundances are different. A number-average mass is used as a quantitative characteristic of the series. It is shown that this value is close for the distributions of the series of compounds in the mass spectrum of exhaled breath condensate and the mass spectrum obtained by summation of direct mass spectra over the breathing time.

Keywords: exhaled breath analysis, exhaled breath condensate, extractive electrospray ionization, smoking

Introduction

Analysis of exhaled breath by mass spectrometry (MS) is an emerging field that may contribute to various areas, such as medicine, pharmaceutics and security. It is noninvasive and has the potential to be a high-throughput, sensitive and specific method for searching and screening biomarkers, drugs and their metabolites, and hazardous compounds.1–4 A series of works devoted to exhaled breath analysis has already proved its usefulness in the search for biomarkers of such diseases as asthma, allergy, cystic fibrosis, cancer etc.1,2,5–7 There are two principal approaches to study exhaled breath composition. The first approach is the analysis of exhaled breath condensate1,8 and the second is a direct analysis of exhaled breath using ambient ionization MS.9–13 The direct analysis is fast and needs no sample preparation, while investigation of exhaled breath condensate allows the application of powerful methods for compound identification, such as liquid chromatography coupled to MS.14,15

The large number of smokers in the world makes it necessary to study the impacts of smoke compounds on the composition of exhaled breath. The smoke contains many compounds of various classes and properties3,4 and provides a strong signal background in exhaled breath. The task of this study is to investigate the molecular mass distributions for a series of compounds that arise in exhaled breath after smoking. Two main approaches are used: direct breath analysis and exhaled breath condensate analysis.