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Volatile organic compounds analyzed by gas chromatography-deep ultraviolet spectroscopy

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ABSTRACT

Exhaled breath contains thousands of volatile organic compounds (VOCs) of which the composition varies depending on status of the individual and the environment. Different metabolic processes within the body produce volatile substances that are released into the blood. When the blood reaches the lungs the products are released into lung tissue and airways.

Also, chronic inflammation and/or oxidative stress can result in the excretion of volatile compounds that generate unique VOC patterns. Therefore, measuring the presence of VOCs in exhaled air (breathomics), for clinical diagnosis and monitoring purposes has gained increased interest over the last years.

This paper describes one methodology based on gas chromatography (GC) and deep ultraviolet (DUV) spectroscopy. Spectra of compounds found in exhaled breath are presented.

1. Introduction

In ancient times, physicians were aware of the relationship between the odour of a subjects' breath and possible diseases associated with it. They realized it could provide insight into physiological and pathophysiological processes in the body [1,2].

It is common knowledge that the sweet acetonic smell of breath might indicate uncontrolled diabetes whereas a fishy reek of breath relates to liver disease and a urine-like smell is associated with kidney failure [3]. Apparently, there is something present in breath that might enable diagnosing certain diseases. Due to the great potential of applications in clinical diagnostics and its non-invasive nature, exhaled air analysis has become of increased interest in recent years.

Exhaled air breath analysis (breathomics) can be applied as an analytical and monitoring tool. In the analytical perspective, VOCs may be used as biomarkers of oxidative stress, inflammation or carcinogenesis [1]. As monitoring tool, breathomics can be applied to elucidate the heterogeneity observed in diseases, to study the pathogen responsible for an infection and to monitor treatment efficacy.

The use of individual VOCs as biomarkers of exposure or disease is hampered by the fact that using a single compound is generally insufficient to monitor complex and heterogeneous processes including environmental exposures or chronic diseases. Therefore, exploring the presence and relations of exhaled VOCs, called the volatome, is expected to generate more adequate information regarding the processes involved. Certainly, analysing the volatome implies a more specific discrimination between various conditions as it reflects changes in both exogenous and endogenous compounds [4–9].

One technique that allows for the detection of the volatome is gas chromatography-deep ultraviolet spectroscopy (GC-DUV). It has been used both for the assessment of environmental factors as well as for individual VOCs [10–17]. However, its use has been hampered by its technical design. In the present study I report on a new design that might allow for the use of GC-DUV on a larger scale.

2. Materials and methods

2.1. Sampling of breath

Exhaled air comprises a mixture of dead-space air and alveolar air. The dead-space air consists of roughly 150 mL air from the upper airway where no gaseous exchange between blood and breath air is facilitated [1,4]. Consequently, this part of the exhaled air displays a high resemblance with the previously inspired air. In contrast, alveolar air originates from the lower airways where gaseous exchange between blood and breath air results in concentrations of endogenous compounds that are two to three times higher compared to those observed in dead-space air. Measuring VOCs in mixed air implies sampling whole breath that consists of both dead-space air and alveolar air. An advantage of sampling 5 L instead of one single breath is a higher reproducibility and lower variability.

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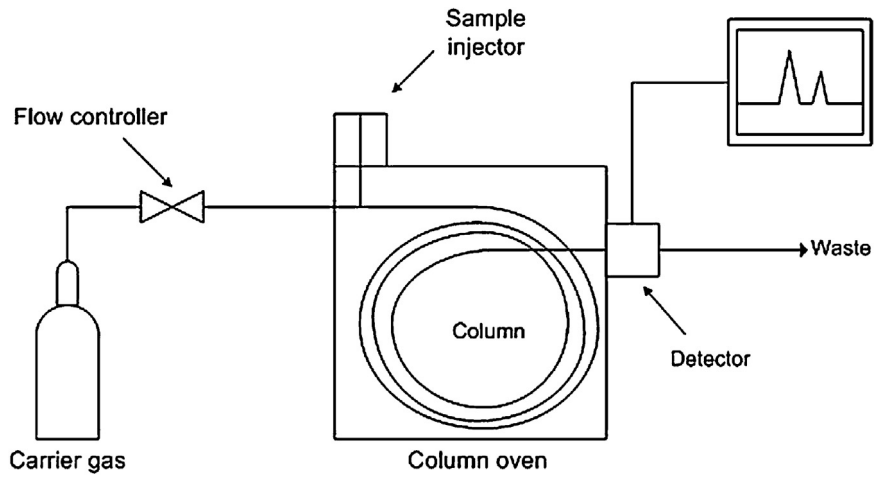

Fig. 1. Schematic illustration of the GC-UV instrumentation.

2.2. Sample preparation technique

In order to collect the compounds present in exhaled air, several technologies are available. Solid-phase microextraction (SPME), is a sample preparation technique used both in the laboratory and on-site. SPME involves the use of a fibre coated with an extracting phase, that can be a liquid (polymer) or a solid (sorbent), which extracts both volatile and non-volatile analytes from different kinds of media such as the exhaled breath collected in a Tedlar® bag. The quantity of analyte extracted (absorbed) by the fibre is proportional to its concentration in the sample as long as equilibrium is reached. After extraction, the SPME fibre is transferred to the injection port of the gas chromatograph (GC), where desorption of the analyte takes place and the separation is carried out. The attraction of SPME is

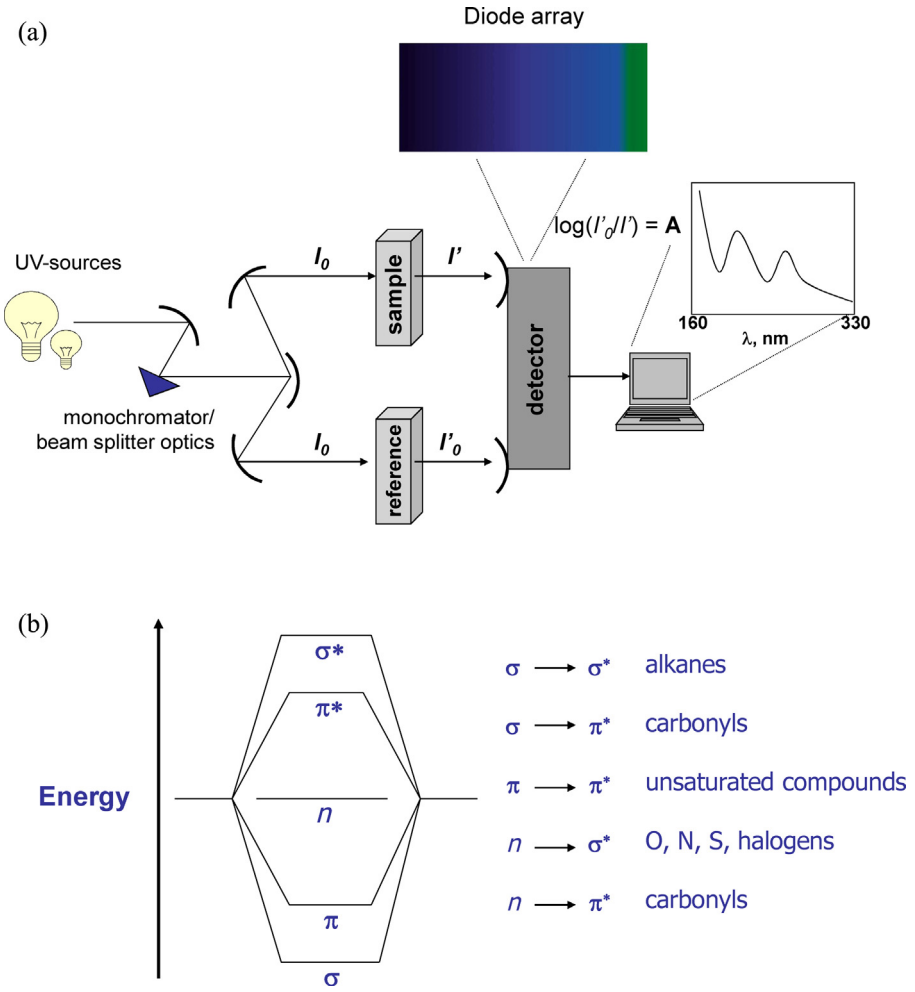

Fig. 2. (a and b) Schematic presentation of the principles of UV spectroscopy.