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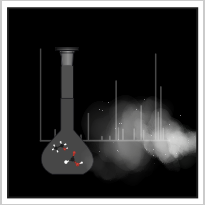

Highlights of Analytical Sciences in Switzerland

Division of Analytical Sciences

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Analysis of Breath-related Volatile Organic Compounds with Laser Absorption Spectroscopy

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Keywords: Extended-tuning quantum cascade laser (QC-XT) · Methanol quantification · On-line breath analysis · Volatile organic compounds (VOCs)

On-line breath analysis has gained much interest in recent years as it has great potential for non-invasive point-of-care diagnostics and personalized medicine. Mass spectrometry is the most frequently used technique, mainly for the untargeted analysis of exhaled breath and the identification of volatile organic compounds (VOCs) as biomarkers. For routine monitoring of established biomarkers, however, there is a need for a method that can provide fast and accurate response in a compact, easy-to-use, and cost-effective instrumentation. Here, mid-infrared laser absorption spectroscopy (LAS) is a promising alternative technique, as already demonstrated by the wide range of monitoring applications, especially for small inorganic gaseous compounds.

Optical analysis of VOCs is, however, far more challenging, because these compounds often exhibit broad, congested, and spectrally overlapped absorption spectra. Consequently, there is a stringent requirement on the laser source to provide broad spectral coverage and high spectral resolution for a selective and accurate multi-VOC analysis.

Our proposed solution to cope with this requirement is the extended-tuning quantum cascade laser (QC-XT). Using this device, we developed a spectrometer that can access six spectral windows spanning over 40 cm^{-1} and provide high-resolution scans (~10^{-4} cm^{-1}) within the individual windows. Custom-built electronics allow rapid switching between and tuning within the six windows (~3300 scans/s), resulting in the measurement of one complete spectrum every 360 ms. With this approach, we can quantify VOCs at amount fractions down to tens of ppb. The broad measuring range and the high spectral resolution of the spectrometer, combined with the unique spectral fingerprints of the investigated VOCs assure excellent selectivity of the method and enable multi-compound measurements in the breath.

This approach allows for the simultaneous measurement of concentration profiles of several VOCs, water vapor and CO_2 in one breath stroke with a relative expanded uncertainty (k = 2) of <2 %.

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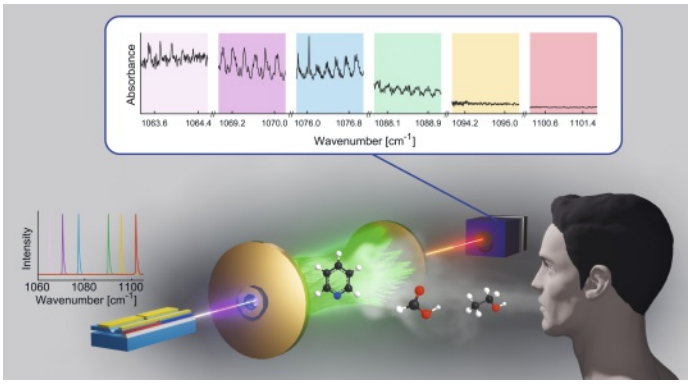
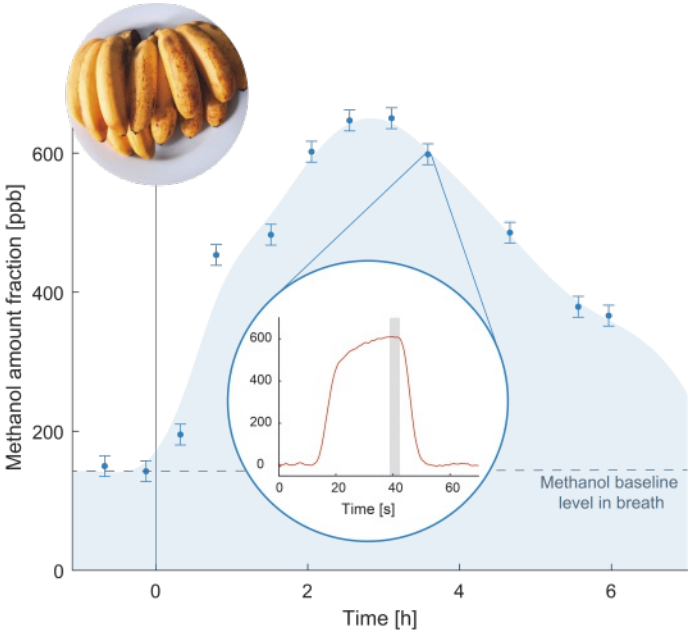


Illustration of the measurement concept. The multi-frequency mid-IR light beam (around 9.25 µm) emitted by the QC-XT laser is coupled into a multi-pass absorption cell (76 m optical path) before reaching the IR detector. A recorded spectrum of pyridine, on top, is shown as a typical example of a broad and congested absorption spectra of VOCs. The spectrometer targets on-line VOC analysis of human breath samples.



Methanol profile in breath before and after consumption of baby bananas measured on-line with the laser spectrometer. Methanol level was expressed as a mean value of measured amount fractions in the last part of a single breath stroke as indicated by the gray bar in the inset.

Reference
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