

# Lung Uptake of Indoor Air Pollutants

*Real-time measurements of VOC uptake into the lungs with Vocus PTR-TOF 2R*

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Breath analysis by online mass spectrometry is emerging as a powerful method to identify potential biomarkers of diseases and to monitor disease evolution and progress of a therapeutic treatment. Mass spectral breath analysis can additionally be used to assess the uptake of molecules from inhaled air into the lungs. This uptake depends on properties such as volatility, solubility, and polarity, with certain compounds more readily passing the blood–air barrier for distribution within the whole body. Accurate estimation of the uptake of a potentially hazardous compound is valuable for risk assessment related to short- or long-term exposure.

Figure 1 shows continuous measurement of inhaled and exhaled air with a Vocus 2R PTR-TOF and a dedicated breath inlet, for a subject in an indoor laboratory space. Time series of acetone, isoprene and N-methyl-2-pyrrolidone concentrations are plotted on a log scale. Acetone and isoprene are common compounds in both ambient air

and human exhalation, as indicated by the increased level during exhalation. N-methyl-2-pyrrolidone is a contaminant originating from the laboratory flooring, which is present in the room air at a concentration of approximately 70 pptv. In contrast to acetone and isoprene, the N-methyl-2-pyrrolidone is consistently less abundant in the exhaled air than in the inhaled room air. This decrease indicates that the compound is taken up in the lungs after inhalation.

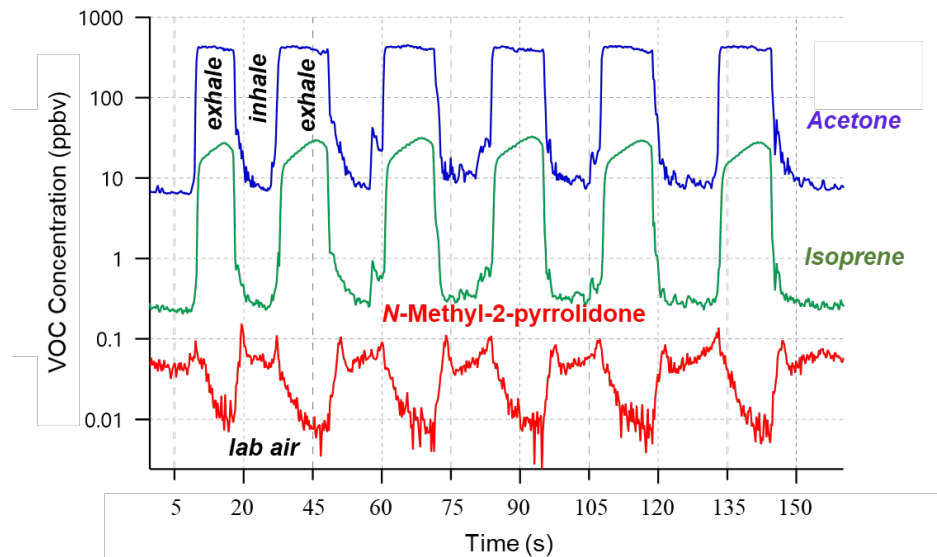
The net uptake of the N-methyl-2-pyrrolidone can be quantified by combining the Vocus data with spirometric information. This is achieved by integrating the difference between ambient concentration and breath concentration of the compound multiplied by the air flow from the lungs, as follows:

$$\int_{t_1}^{t_2} [C(t) - C_{lab}] f(t) dt$$

where  $t_1$  and  $t_2$  are the time of the beginning and the end of the measured breath exhalation, respectively;  $C(t)$  is the

compound concentration measured by Vocus during the exhalation;  $C_{lab}$  is the laboratory concentration of the compound; and  $f(t)$  is the breath air flow

during the exhalation. Such calculation leads to an estimation of 150 ng / breath of N-methyl-2-pyrrolidone uptake into the lungs.



**Figure 1.** Analysis of human breath at 5 Hz by a TOFWERK Vocus 2R PTR-TOF over a period of 10 minutes. The subject inhales air from the laboratory and exhales into the breath inlet of the instrument. The time evolution of acetone (blue), isoprene (green) and N-methyl-2-pyrrolidone (red) are reported. The latter is an air contaminant originating from the laminate used in the laboratory flooring and is always present. In these data, its concentration is consistently higher in the inhaled air and lower in the exhaled air, indicating uptake of the compound in the lungs.

## Contact

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 tofwerk.com/products/vocus-ptr-tof/  
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