Examination of Sampling Bags for Offline Breath Analysis using Secondary Electrospray Ionization (SESI) Mass Spectrometry

M. Fido[1], S. Giannoukos[1], R. Zenobi[1]*

[1]Department of Chemistry and Applied Biosciences, Swiss Federal Institute of Technology, Zürich, Switzerland

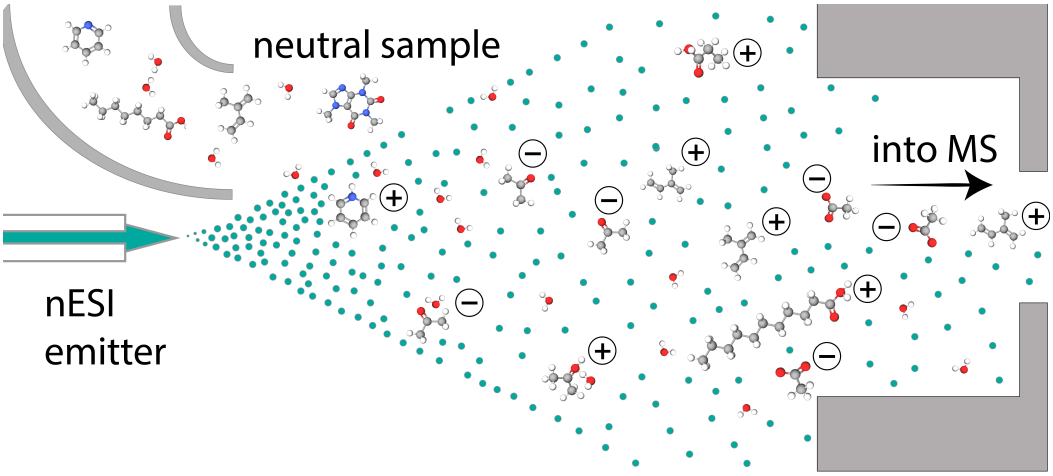
Research on exhaled breath, a fast-developing area of metabolomics, focuses on identifying disease biomarkers, tracking nutritional interventions, and analyzing the human volatilome.[1,2] It is a non-invasive, reliable and sensitive approach to diagnostics with the potential to replace invasive methods, such as blood sampling. Online analysis is the method of choice for breath analysis; however, in the clinical setting, access to a measurement facility is often limited, especially for bedridden patients. In these situations, offline methods are a viable alternative. Sampling bags are one of the most common offline sampling methods for exhaled breath.

Secondary electrospray ionization focuses on introducing an ambient gaseous sample into the ion source, where it collides with a charged nano-electrospray. The analyte molecules are subsequently ionized in the gas phase without any sample preparation or preconcentration. This approach works online and offline and is sensitive to the low-ppt range, making it a robust tool for exhaled breath analysis.[3]

In this work, we present the use of SESI coupled to a high-resolution mass spectrometer for rapid analysis of breath samples stored in bags made from various materials: Tedlar (PVF), Teflon (PTFE), Nalophan (PET), Kynar (PVDF) and EVOH (ethylene vinyl alcohol copolymer). We investigated a number of qualitative properties, such as retrievability of common breath markers, the total number of features and impurities found within each bag material.

Acknowledgements

We thank the ETH Zürich Foundation and the Departmental Mechanical Workshop for supporting this work.



References

[1] Mansurova M. *et al. Current Genetics,* **2017**, 64, 959-964.
[2] Wüthrich Cedric., *et al.*, *Journal of Breath Research,* **2022**, 16 (4), 046007.
[3] Bruderer Tobias, *et al.*, *Chemical Reviews,* **2019**, 119, 10803–28.