39th Informal Meeting on Mass Spectrometry
Paris, France, May 15-17, 2023

Chemical ionization in a compact FT-ICR mass spectrometer for real-time analysis of pathological biomarkers in sweat

T. ABAR[1)], *H. MESTDAGH*[1)], *J. LEMAIRE*[1)] *and M. HENINGER*[1)]

1) *Institut de Chimie Physique UMR8000 - Université Paris-Saclay, 15, avenue Jean Perrin, 91405; Orsay, France*

Health issues are a significant problem for our societies. Early diagnosis can significantly contribute to a decrease in mortality caused by diseases. In this respect, a non-invasive and rapid medical analysis would be a promising alternative to the usual clinical diagnostic methods requiring invasive sampling and/or extended biomedical analysis. It would provide access to disease-specific biomarkers with minimal inconveniences. It has been known for a long time that some diseases can change the body odors by emitting various substances, classified as VOCs (Volatile Organic Compounds), in the different biological fluids (urine, sweat, blood, exhaled breath….). Identifying some of these VOCs in biological matrices is an exciting project that presents new challenges. The main objective of my thesis is to develop an analytical device based on mass spectrometry to analyze sweat samples and identify volatile biomarkers characteristic of diseases.

In the present work, we used an FT-ICR mass spectrometer with a permanent magnet coupled to chemical ionization and a tubular furnace for real-time analysis of isovaleric, lactic, pyruvic acids, and urea. The presence of those molecules at high concentrations (mM) in sweat indicates a health problem related to isovaleric acidemia [1], pressure ischemia [2], and/or kidney failure [3].

Test analyses are performed as follows: sample solutions were soaked on a sterile gauze, vaporized by heating in the furnace, and introduced in the mass spectrometer to be analyzed under controlled conditions.

For this purpose, several parameters were optimized, such as i) the heating program of the furnace, ii) the flow of the carrier gas iii) the device allowing sample introduction in the mass spectrometer: three-way or two-way valve. Those optimizations were performed with 100 ppm in mass toluene aqueous solution.

Results will be shown on analysis of aqueous solutions of the four biomarkers, first individually, then as a mixture, at different concentrations.

References

1. M. Shirasu, K. Touhara; The Journal of Biochemistry., 150 (3), 257–266 (2011)
2. J. Derbyshire, H. Barr, F.Davis, S. Higson; J Physiol Sci., *62* (6), 429–440 (2012)
3. Z. Sonner, E.Wilder, J. Heikenfeld, G. Kasting, F. Beyette; Biomicrofluidics., 9 (3), 031301 (2015)