Early stage non-invasive diagnostic of diseases can possibly take place by analyzing volatile organic compounds (VOCs) released from the breath of patients [1]. Breath VOC samples are typically analyzed using one dimensional (single-column) gas chromatography coupled to mass spectrometry (1DGC-MS). In that context, a limited number (< 50) of VOCs (mainly alkane and benzene derivatives) has been identified as potential biomarkers of disease in breath VOC profile.

Because of the complexity of breath VOC mixtures, it is believed that more biomarker candidate could be found. Comprehensive two-dimensional GC coupled to time-of-flight mass spectrometry (GC×GC-TOFMS) is a powerful separation science tool and has been successfully used to separate more than one thousand of VOCs in human breath [2].

In addition to the large peak capacity, latest advances in GC×GC-TOFMS data processing tools also allows better handling of the interfering environmental VOCs to the breath signature. Supervised statistics can be applied to the GC×GC chromatograms in either a peak table-based or a pixel-based approach [3,4]. Inter-individual variations and sampling effects can therefore be minimized in order to improve the isolation of specific molecules.

In this paper, we report on practical examples of such specific data treatment procedures in the case of lung cancer screening by means of breath sampling of patients at the time of bronchoscopy.


