

GCxGC-TOFMS and SIFT-MS approaches for clinical breath-based asthma phenotyping

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Abstract

The ballistic rise of analytical technologies has opened a large playground for all type of “omics” screening. On one side, separation science based on multidimensional methods such as comprehensive two-dimensional gas chromatography (GCxGC) appeared as one of the methods of choice for the characterization complex mixtures. On the other side, direct introduction instruments such as single ion flow tube mass spectrometry (SIFT-MS) offered the capacity to perform both targeted and non-targeted analyses within a few minutes. At the price of high cost equipment and limited adaptability to routine medical usage, GCxGC-HRTOFMS offers the possibility to almost completely characterize a sample composition. This is of prime importance when systems biology are considered. For large scale screening, SIFT-MS can generate compositional patterns from direct sample introduction at the same time than other routine medical actions. These two orthogonal approaches for pathology screening should ideally conduct to identical sample classifications but have never been directly compared over an identical set of patients.

In this study, breath from 50 asthmatic patients were analyzed by both techniques. As a reference, asthma phenotypes were established using sputum analysis. Breath samples were collected using Tedlar® bags. For GCxGC-HRTOFMS analyses, the bags were transferred onto thermal desorption tubes prior to injection. For SIFT-MS, the bags were directly emptied into the instrument. Next, data were analyzed using identical processing workflow. We observed that both approaches offered similar classification capacities. GCxGC-HRTOFMS allowed identifying the putative markers for comparison with previous studies and metabolic interpretation while SIFT-MS offered a faster screening capacity.