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METHOD DEVELOPMENT AND OPTIMIZATION FOR MONITORING PROBE EXHALED BREATH METABOLITES USING PARALLEL MS-BASED ANALYTICAL PLATFORMS

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Abstract

The high potential of exhaled breath for disease diagnosis has been highlighted in numerous studies. However, exhaled breath analysis is suffering from a lack of standardized sampling and analysis procedures, impacting the robustness of inter-laboratory results, and thus hampering proper external validation. The aim of this work was to verify compliance and validate the performance of two different comprehensive two-dimensional gas chromatography coupled to mass spectrometry platforms in different laboratories by monitoring probe metabolites in exhaled breath following the Peppermint Initiative guidelines. An initial assessment of the exhaled breath sampling conditions was performed, selecting the most suitable sampling bag material and volume. Then, a single sampling was performed using Tedlar bags, followed by the trapping of the volatile organic compounds into thermal desorption tubes for the subsequent analysis using two different analytical platforms. The thermal desorption tubes were first analyzed by a (cryogenically modulated) comprehensive two-dimensional gas chromatography system coupled to high-resolution time-of-flight mass spectrometry. The desorption was performed in split mode and the split part was recollected in the same tube and further analyzed by a different (flow modulated) comprehensive two-dimensional gas chromatography system with a parallel detection, specifically using a quadrupole mass spectrometer and a vacuum ultraviolet detector.