Comparison of different GC-IMS-Devices for Measurement of volatile Biomarkers (VOC)

G. Becher[1,2,] R. Purkhart[3], Anne Hillmann[4], R. Graupner[2], W. Schüler[5]
[1]BecherConsult GmbH, Bernau, [2]Graupner GmbH & Co KG, Geyer, [3]IFU Institut für Diagnostik, Oberlichtenau, [4]Hochschule Mittweida, [5]STEP Sensortechnik, Pockau,

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Introduction

The Ion Mobility Spectrometry (IMS) is a highly sensitive analytical method for detection of volatile organic compounds (VOCs) in air. Available studies were typically done with one device in mono-centric studies only. The aim of the study was the comparison of different devices. The study was done as basis for detection of bacterial growth in standardized cultures of MAP.

Methods

The headspaces of in vitro cultures of two strains of *mycobacterium avium* were measured with a GC-differential-ion-mobility-spectrometry (DMS-SIONEX) as well as with a GC-IMS Prototype (GC-IMS) 1 week after inoculation. Pure breeding grounds were measured as control. Sample collection was done by internal suction pump and rinsing of the tubes with filtered air. The spectra were analyzed by a statistical program based on cluster analysis and non-parametric statistics (U-test).

Fig. 1: Laboratory Setup

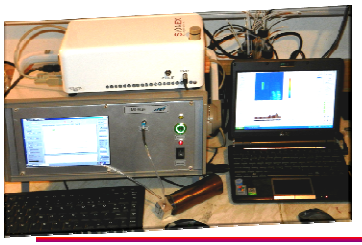
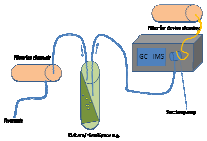


Fig. 2: Sample-collection



Results

Both devices show spectra with comparable numbers of peaks. It was possible to perform a significant differentiation between pure agar and the bacterial growth. Each cluster represents the same peaks, e.g. detected metabolite, in the different culture-tubes.

Fig. 3: Heatmap of Breeding Ground

DMS GC-IMS

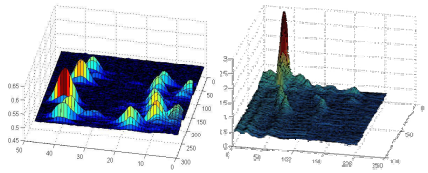
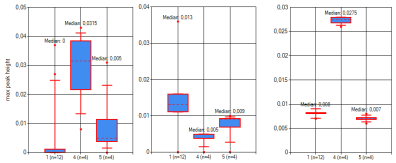


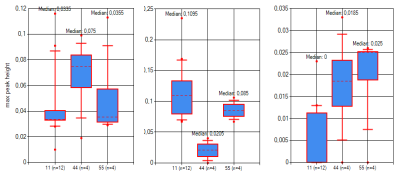
Fig. 4: Heatmap and identified clusters for differentiation of MAP-growth on breeding ground: [1] pure agar; [4] original count.; [5] 10^{-4} dilution of bacterial count.

DMS



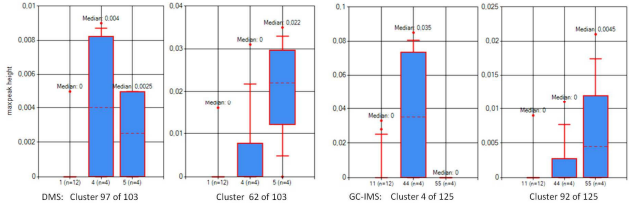
Cluster 67 Cluster 20 Cluster32

GC-IMS



Cluster 18 Cluster 3 Cluster 24

Fig. 5: Clusters which enables the differentiation between pure medium [1] and MAP-strain 1 [4] and MAP-strain 2 [5] for both devices.



Discussion

With both devices the differentiation between breeding ground and bacterial growth was possible with a sensitivity and specifity of 100%, using two to three clusters. Additionally other clusters ensure the differentiation between the two strains.

GC-IMS may be a more rapid tool for detection of bacterial growth in vitro than traditional methods. Different IMS-Devices, i.e. different pre-settings of the devices gave comparable results. By knowledge of the positions of peaks of similar substances the use of different device-settings is no impediment for multicentric studies.

The possible inclusion of a couple of clusters increase the significance. The lack of knowledge about the chemical structures of clusters will not prevent the meaningfulness of the differentiation of groups. Great learning engraving samples will improve the statement and allow a clinical application within short term.

[1] R. Purkhart , A. Hillmann, R. Graupner, G. Becher: Detection of characteristic clusters in IMS-Spectrograms of exhaled air polluted with environmental contaminants. IJIMS, Feb. 2012 (DOI 10.1007/s12127-012-0090-4)
[2] R. Purkhart: Klassifikation von Ausatemluft anhand ihrer differenziellen Ionenbeweglichkeitsspektrogramme. Diplomarbeit, HUB 2010
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Kontakt: Gunther Becher
info@becherconsult.de