Large Scale Scanning of Metabolites in IMS-Chromatograms

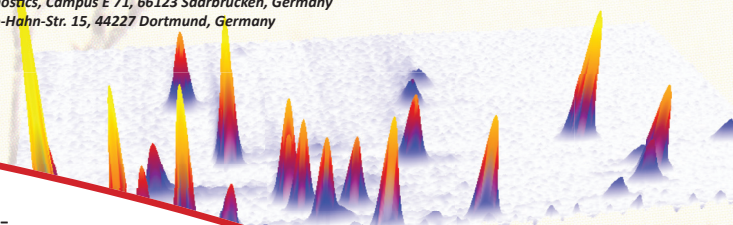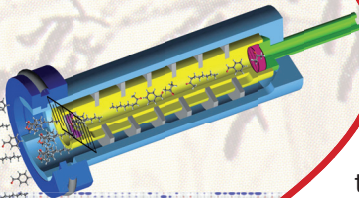## S. Maddula[1], K. Rupp[1], J.I. Baumbach[1,2]

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Part of a IMS-Chromatogram of human breath

Ion mobility spectrometry coupled to a multi-capillary column (MCC/IMS) was introduced for medical applications including intensive care and point of care to detect signals related to bacteria, cancer, diseases, inflammation, pharmaceuticals etc. Not only the analytical questions such as sampling, sample introduction and operation are gaining significance, but also various data mining operations are attaining increased importance. The parallel evaluation of some hundreds of peaks characterized by position, volume, and consideration of monomers, dimers and trimers, and searching in databases with thousands of data from patients needs standardization and efficien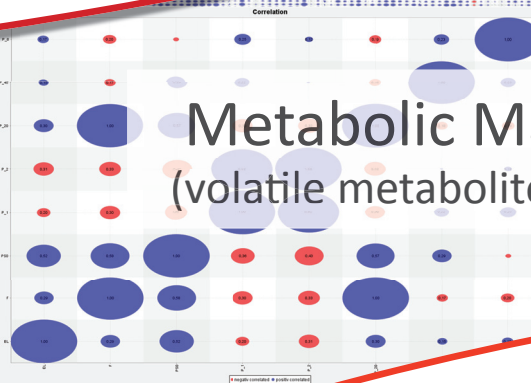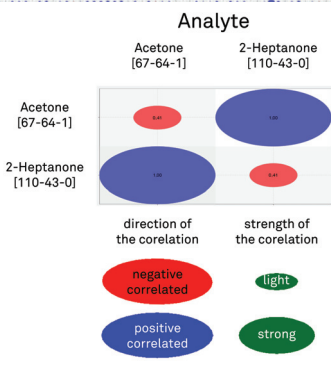t data mining procedures. Validation of analytes e.g. using parallel GC/MSD measurements makes the situation more complicated.

ANALYTES →

Metabolic Map of a Patient
(volatile metabolites in exhaled breath)

Analyte

Acetone [67-64-1] | 2-Heptanone [110-43-0]

Acetone [67-64-1]
2-Heptanone [110-43-0]

direction of the corelation | strength of the corelation

- negative correlated
- positive correlated
- light
- strong

Actually, two different software packages were developed with respect to visualization of IMS-Chromatograms and including peak identification, referencing and classification with respect to large scale applications. The software package IPHEX (by A. Bunkowski, Bielefeld, Germany) focuses on handling of data and supports manual search for peaks and relations to classes of diseases including bar charts and box-and-wisker plots. On the other hand, VisualNow (by B. Bödeker, B&S Analytik, Dortmund, Germany) focuses on automatic large scale scanning of IMS-Chromatograms and includes preparation of reports based on rank sum, box-and-wisker plots and probability densities of relevance.

- Pseudomonas
- Control

P_1 / PS0

Control | Pseudomonas

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