

Large Scale Scanning of Metabolites in IMS-Chromatograms

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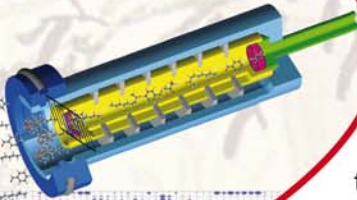
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Ion mobility spectrometry coupled to a multi-capillary column (MCC/IMS) was introduced for medical applications including intensive care and point of care to detect signals related to bacteria, cancer, diseases, inflammation, pharmaceuticals etc.

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 efficient data mining procedures. Validation of analytes e.g.

using parallel GC/MSD measurements makes the situation more complicated.

Part of a IMS-Chromatogram of human breath



ANALYTES

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

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.

Acknowledgements

The financial support of the Ministry of Education, Science and Technology (MEST) of the Republic Korea is acknowledged thankfully. Part of the work on this paper has been supported by Deutsche Forschungsgemeinschaft (DFG) within the Collaborative Research Center (Sonderforschungsbereich) SFB 876 „Providing Information by Resource-Constrained Analysis“, project TB1 „Resource-Constrained Analysis of Spectrometry Data“.

In addition, the work was supported partly by the German Federal Ministry of Economics and Technology based on a decision of the German Bundestag within the project KF2368102AKO.

The authors thank K. Darwiche, U. Sommerwerck and L. Freitag among other colleagues of the Ruhrlandklinik Essen for release of the data obtained in Essen.

Analyte

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

