

Machine Learning Approaches to identifying Volatile Organic Compounds

Background

Diabetes mellitus is a chronic metabolic disorder affecting millions worldwide. Continuous monitoring of diabetes is crucial for effective management and prevention of complications. Emerging research suggests that changes in volatile organic compounds (VOCs) present in breath could provide valuable insights into metabolic processes associated with diabetes. Specialized instruments such as gas chromatography-ion mass spectrometers (GC-IMS) can measure the presence and concentration of VOCs in breath. The analysis of VOCs offers a non-invasive and potentially rapid means of monitoring diabetes-related metabolic fluctuations. However, the complex and diverse nature of VOC patterns necessitates advanced analytical methods.

Aim

This research aims to develop a machine learning-based approach for the analysis of volatile organic compounds in breath, with the goal of identifying distinctive VOC patterns associated with metabolic states (glucose levels) in diabetes.

Materials and Methods

For this project, the student will analyse data from a clinical study that were taken with the BreathSpec device (GC-IMS). First, the student will use data preprocessing algorithms to perform noise reduction and feature extraction. Then the student will employ classification and clustering models, to identify distinctive VOC patterns in breath associated with low and high blood glucose levels in diabetes. The work will involve collaboration with medical experts to ensure clinical relevance and accuracy.

Nature of the Thesis:

- Literature research: 10%
- Experimental: 10%
- Data and image processing and programming: 70%
- Documentation: 10%

Requirements:

- Motivation to work in a multidisciplinary team
- Programming skills in python for data processing and AI

Supervisors:

Prof. Dr. Lilian Witthauer
Prof. Dr. José Garcia

Institutes:

Department of Diabetes, Endocrinology,
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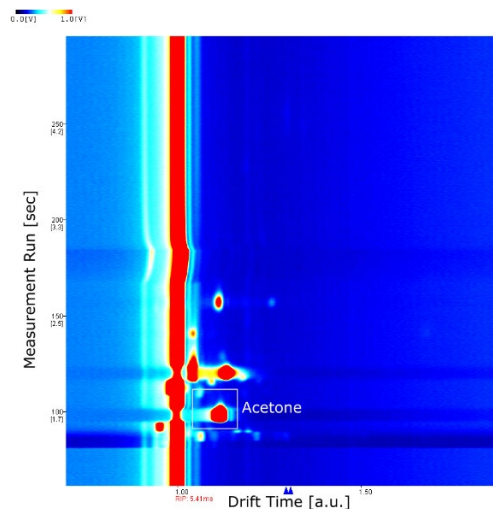


Fig. Breath analysis using GC-IMS.