Bioinformatics Methods for Breath Analysis and Biomarker Detection

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Abstract:

The volatilome is the sum of volatile organic compounds that are emitted by all living cells and tissues. We seek to non-invasively "sniff'" biomarker molecules that are predictive for the biomedical fate of individual patients. This promises great hope to move the therapeutic windows to earlier stages of disease progression.

While portable devices for breathomics measurement exist, we face the traditional biomarker research barrier: a lack of robustness, which hinders translation to the world outside laboratories. To move from biomarker discovery to validation, from separability to predictability, we have developed several bioinformatics methods for computational breath analysis, which have the potential to significantly boost non-invasive biomedical decision making by rapid and cheap matching of decisive patterns in exhaled air. We aim to provide a supplementary diagnostic tool complementing classic urine, blood and tissue samples. The presentation will review the state of the art, highlight existing challenges and introduce new data mining methods for identifying breathomics biomarkers.

Relevant Publications:

Schneider T, Hauschild AC, Baumbach JI, Baumbach J (2013) An integrative clinical database and diagnostics platform for biomarker analysis in ion mobility spectra of human exhaled air. J Integr Bioinform. 2013 Apr 2;10(2):218.

Hauschild AC, Kopczynski D, D'Addario M, Baumbach JI, Rahmann S, Baumbach J. Peak detection method evaluation for ion mobility spectrometry by using machine learning approaches. Metabolites. 2013 Apr 16;3(2):277-93.

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Maurer F, Hauschild AC, Eisinger K, Baumbach J, Mayor A and Baumbach JI. MIMA - a software for analyte identification in MCC/IMS chromatograms by mapping accompanying GC/MS measurements. Int. J. Ion Mobil. Spec. 2014 Apr:17:95–101.

Smolinska A, Hauschild AC, Fijten RR, Dallinga JW, Baumbach J, van Schooten FJ. Current breathomics-a review on data pre-processing techniques and machine learning in metabolomics breath analysis. J Breath Res. 2014 Jun;8(2):027105.

Hauschild AC, Schneider T, Pauling J, Rupp K, Jang M, Baumbach JI, Baumbach J (2012) Computational methods for metabolomics data analysis of ion mobility spectrometry data - Reviewing the state of the art. Metabolites 2012, 2, 733-755.