



Master of Science – Biomedical Engineering
Thesis Proposal

Evaluating the impact of batch effect in SESI-HRMS data and compare different batch correction methods

Breath analysis by secondary electrospray ionization high-resolution mass spectrometry (SESI-HRMS) has potential for clinical diagnosis and drug monitoring. SESI-HRMS offers a number of advantages (e.g., real-time, yet wide, metabolome coverage) that makes it ideal for untargeted and targeted studies. In past few years we have developed standard operating procedures (SOP) to perform stable and reproducible SESI-HRMS experiment in monocenter [[Singh and Tancev et al., 2019](#); PMID: 30989265] and multicenter setting [[Gisler and Singh et al., 2022](#); PMID: 36479147]. However, despite adhering to our SOPs, like any other omics technique we have also observed batch and/or effects. In the past, we used well established batch correction methods to deal with these effects.

The aim of this master thesis would be to explore the impact of different types of batches (including site) on the existing high-quality SESI-HRMS data and to evaluate and compare and different batch correction methods. Additionally, experimental possibility to tackling batch effect at the data acquisition level will also be explored. This work will bring SESI-HRMS one step closer to being utilized in multicentric studies.

Nature of the Thesis

Programming and data analysis: 50 %
Experimental: 30 %
Documentation: 20 %

Specific Requirements

Programming experience in MATLAB and R.
Genuine interest in a highly interdisciplinary project.

Supervisor

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