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ESTABLISHING AN GC-MS BASED METABOLOMICS PLATFORM

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Metabolomics has become a powerful tool to study processes in organisms and to identify biomarkers. In recent years, within the Research and Innovation Centre (CRI) at Edmund Mach Foundation (FEM) a mass spectrometry (MS) based technological platform for high throughput metabolomics has been set up, with the objective of analysing different sample types (including plant tissue like fruits, leaves, roots but also urine, faeces, liver, kidney samples).

For analysis of volatiles we use a gas chromatography (GC)-MS system with an autosampler solid phase microextraction (SPME) device. Optimisation of SPME parameters is crucial to detect as many metabolites as possible and these parameters are sample dependent. Hence, we established an SPME parameter optimisation method based on an D-optimal design. This requires only a rather low amount of injections to identify SPME conditions providing the highest number of peaks. The input to the D-optimal design is provided by an automated and unbiased peak picking process using the xcms [1] R package. Within the data analysis pipeline, feature annotation and substance identification is performed by combining xcms with in-house developed software solutions, which rely on commercial and in-house mass spectra libraries.

Quality control is of high importance for all the high-throughput metabolomic applications. With our workflow, it is ensured by the regular injection and analysis of specific quality control (QC) samples.

This presentation shows the platform setup and its application to grape samples.

References

[1] C.A. Smith *et al*., Analytical Chemistry 78 (2006) 779