

From profiling to biochemical insights - Bioinformatics & Mass Spectrometry

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Mass spectrometry is an important analytical technology in metabolite profiling. The first steps of the analysis pipeline for MS measurements are signal processing and peak picking tasks. We are actively developing and enhancing the open-source software XCMS and related bioconductor packages.

The next step in bioinformatics is the statistical analysis, checking e.g. for significant differences between samples even in the presence of high biological variation. This can reveal "interesting" features, and subsequent tandem MS experiments provide powerful structural hints for the elucidation of these unknown mass spectral features.

Using data from modern mass spectrometers it is possible to combine both steps with our MetFamily tool and seamlessly navigate between statistical analysis and structural characterisation of metabolites.