

OW5 MS Metabolomics – from biomarker discovery to rapid class targeted analysis

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Ion trap mass spectrometry (MS) is a powerful tool for unbiased and targeted metabolomics.

Mass spectrometry is a key technology for metabolomics research. Described are two MS metabolomics studies, one based on biomarker discovery and the other on rapid and sensitive class-targeted analysis.

Phylloxera is a serious wine industry pest leading to productivity loss and even vineyard replanting. Phylloxera, a small subterranean insect, may be well established in a vineyard before being detected by overt symptoms of vine stress and confirmatory root excavation. Initial metabolomic studies for the early detection of phylloxera via LCMS analysis of vine leaves reveal the level of certain metabolites, including flavanols, are significantly upregulated (2-4 fold) in the presence of the insect.

Glucosinolates are naturally occurring anionic secondary plant metabolites incorporating a thioglucosidic link to the carbon of a sulphonated oxime. These metabolites are of interest for both their anticancer and flavour properties. Parent ion mapping is an analytical mass spectrometry approach allowing assessment of glucosinolate content. Ion mapping is rapid (2-3 minutes) and sensitive (ng/L). This method takes advantage of the glucosinolate anion fragmentation which consistently produces a sulphonate ring-opened glucose moiety via an intramolecular transfer mechanism. This fragmentation can be exploited as a general identifier of the glucosinolate class in plants and LCMSⁿ can provide positive identification and quantification of individual glucosinolates. Such approaches offer sensitive tools for focused metabolomics analysis and screening of plant breeding lines.