NMR- and UHPLC-MS-based metabolomics for the discrimination of different resistant *Vitis vinifera* cultivar woods.

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*Vitis* cultivars exhibit different susceptibility to pathogens such as *botrytis* or downy mildew and the selection of resistant species is important for a sustainable wine production without use of harmful pesticides. In order to highlight biomarkers that can be related to *Vitis* resistance to common diseases, woods of resistant *vitis* cultivars were profiled by NMR and UHPLC-TOF-MS [1] and analysed by chemometric methods utilizing both NMR and UHPLC-TOF-MS data [2], using Statistical HeterospectroscopY (SHY) while furthermore, the Statistical Total Correlation Spectroscopy (STOCSY) was applied in the NMR dataset for identification of the critical metabolites found in the NMR spectra. Three different samples of *Vitis* wood, one resistant to *botrytis*, one resistant to downy mildew and one susceptible to both phytopathogenic microorganisms were used in this study. The wood samples of specific specimens were divided in 18 groups (6 per cultivar) and extracted separately with EtOAc to offer statistical confidence. Two different sample preparation protocols were developed and applied in parallel for the NMR (600 MHz) and UHPLC-TOF-MS analysis of the extracts, respectively. Multivariate data analysis using both supervised (PLS-DA) and unsupervised (PCA) methods revealed a clear distinction between the three groups as well as in the discrimination between the two different resistant species. A high convergence regarding the discrimination patterns between NMR and UHPLC-TOF-MS data was obtained. The NMR and MS variables derived from the loading plots were attributed to specific biomarkers, which were further evaluated by STOCSY. This statistical model could be efficiently applied for the determination of resistant cultivars of *Vitis* as well as for the identification of novel biomarkers involved in resistance phenomena.

References