SELECTED ION FLOW TUBE MASS SPECTROMETRY: A PROMISING TECHNOLOGY FOR THE HIGH THROUGHPUT PHENOTYPING OF GRAPE BERRY VOLATILOME

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Abstract:

Context and purpose of the study - Wine grapes breeding has been concentrating a lot of efforts within the grape research community over the last decade. The quick phenotyping of genotype quality traits including aroma composition remains challenging. Selected Ion Flow Tube Mass Spectrometry (SIFT-MS), a technology first available in 2008 and developing rapidly, could be particularly valuable for this usage. The aims of this study were i) to use SIFT-MS, to analyze the whole volatilome from different grape varieties, ii) to assess the ability of this technology to discriminate varieties according to their grape aroma composition, and iii) to study the stability of SIFT-MS signal over maturation to define a sampling strategy.

Material and methods - 23 grape varieties were sampled at 40 days after mid-veraison in a germplasm collection, and 50 g of berries were subsampled and crushed to be directly analyzed in the SIFT-MS using H_3O^+, NO^+ and O_2^+. Straightforward chemometrics techniques such as ANOVA and PCA were used to analyze spectral data and select discriminant masses. For each homogenous group of cultivars made using hierarchical clustering analysis (HCA), one grape variety was chosen to perform analyzes by gas chromatography–mass spectrometry (GC-MS) to associate masses found in the SIFT-MS and compounds in the NIST database library. At the same time on a neighboring vineyard, samples of Syrah were collected at 7 times between mid-veraison and 50 days after mid-veraison.

Results - Based on their SIFT-MS volatilome scan, different grape variety groups could be identified. O_2^+ reagent ions should be given preference due to their propensity to ionize the majority of compounds, effectively fragment them to produce ions with distinct *m/z* ratios, and improve the distinction of compounds with comparable masses. As demonstrated by headspace GC-MS investigations, the technique permitted the differentiation of high and low aroma compound producers. Analyzes performed on Syrah berries highlighted the stability of SIFT-MS volatilome from 28 days after mid-veraison.

SIFT-MS has proved to be an interesting instrument, enabling a rapid analysis of berry aroma composition in less than 3 minutes with O_2^+, with potential and already transposable applications in many viticultural areas, including the phenotyping of grape varieties or the untargeted study of the effect of viticultural practices. For phenotyping, berries shall be collected from 28 days after mid-veraison, a time point allowing signal stability.

Keywords: SIFT-MS, Grapes, Volatilome, Phenotyping, Breeding, Statistical pipeline.