Searching for the most variable *m/z* values in grape development in a Portuguese vineyard

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Each vineyard is known to have a strong impact on the metabolic compounds of grapes due to its external factors, named *terroir* [1]. Furthermore, knowledge on the metabolic behavior of vines in response to the *terroir* effect can help to assess, in advance, the optimal maturity of grapes. The aim of this work was to obtain a metabolic profile of vines in different locations and consequently associate it with the external conditions present during grapes' development using an untargeted approach.

Samples were collected in eight sites of a Portuguese vineyard during different developmental stages and analyzed using a metabolomic protocol based on liquid chromatography coupled to tandem mass spectrometry [2]. Briefly, samples were grounded and extracted using a mixture of water/methanol/chloroform (20:40:40, v/v/v). The aqueous methanol fraction was used for further analysis. An Agilent Eclipse plus C18 column (RRHD 1.8 μm, 2.1 mm × 100 mm) was used for chromatographic separation and elution was achieved in gradient mode. Water and acetonitrile both containing 0.1% (v/v) formic acid were used as mobile phase. Mass spectrometry analysis was performed in positive and negative ionization mode and data were acquired in scan mode to maximize the number of detected *m/z* values. MZmine software was chosen for data analysis due to its robustness in fragment selection. A baseline correction was applied to equalize baselines and an alignment algorithm was used to equalize retention times aiming to compare *m/z* values from different samples. Statistical and chemometric tools were used to exclude *m/z* values attributed to blanks and to establish a metabolic profile, respectively.

Preliminary results confirm that the methodology chosen for data analysis is fast and accurate for the viable selection of the most significant *m/z* features. Regarding currently analyzed samples, the proposed methodology allowed the identification of several *m/z* features presenting a statistically significant variation among sampling points, which will be further investigated as indicators of the maturity state.

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