LC-MS based metabolomics discriminates premium from varietal chilean Cabernet Sauvignon cv. Wines

Aim of the study was to investigate the metabolomic differences between Chilean Cabernet Sauvignon wines, divided according to their quality in two main groups: "Varietal" and "Premium", and to point out metabolites tentative markers of their chemical signature and sensorial quality. Initially, 150 (50 x 3 biological replicates) experimental wines were produced by the same semi-industrial process, which covered 8 different Chilean valleys. The wine classification made by experts, divided the wines into two major groups ("Varietal" and "Premium") and four subgroups (two for each major group). All the samples were analyzed according to a robust LC-MS based untargeted work-flow (Arapitsas et al 2018), and the proposed minimum reporting standards for chemical analysis of the Metabolomics Standards Initiative (Sumner et al 2007). The produced big-dataset was based on 7633 features for ESI- mode analysis and 9258 for ESI+ mode. After the quality control of the data, were found 150 tentative markers. The annotation of the markers was achieved by using the internal library, external databases and literature information. Between the Chilean Cabernet Sauvignon quality tentative markers were annotated N-compounds (e.g. peptides), stilbenoids, flavanols, anthocyanins and sulfonated compounds. In conclusion, this study allowed us to find metabolomic pathways and chemical reactions, and therefore propose new hypothesis, which could open new frontiers for the understanding of the Chilean Cabernet Sauvignon quality and terroir effect and provide new tools for the enology of precision in Chile.

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