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LUPULIN GLANDS MICROSAMPLING: NEW APPROACH FOR HOPS METABOLOMIC FINGERPRINT EXPLORATION

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Hops (*Humulus lupulus* L.) have been used for centuries in beer production, primarily due to lupulin, a resin with a complex chemical composition found in the lupulin glands in the inflorescences. Lupulin glands are glandular trichomes responsible for biosynthesizing secondary metabolites that confer the plant's characteristic properties, whereas the surrounding plant tissue, supposedly, contributes minimally to hop chemical traits. Several studies on the plant species have predominately focused on analyzing the inflorescence as a whole, since in beer production entire inflorescences are used (i.e., they are not separate into different types of plant tissue). Consequently, studies that investigate the chemical composition of trichomes are rare. Even more scarce are studies of trichomes originated from tropically grown hops. This study aimed to analyze the metabolic fingerprint of glandular trichomes from hops cultivated in tropical regions using microsampling as a sampling technique. The plants were grown in six regions in the states of São Paulo and Minas Gerais and analyzed using liquid chromatography coupled to mass spectrometry followed by unsupervised and supervised multivariate statistical analysis (Principal Component Analysis - PCA and Partial Least Squares Discriminant Analysis - PLS-DA). Samples from two commercial hop cultivars (Cascade and Comet) were evaluated. The samples included isolated trichomes, inflorescence extracts, and imported pellets (Germany). Chromatograms obtained from the trichomes revealed the methodology suitable for metabolic studies, presenting clear, well-defined picks, and similar pattern to previous studies utilizing hops extracts from the whole inflorescence. PCA (R^2X 0,872 e Q^2 0,825) displayed the data for all samples in two non-overlapping clusters. One containing trichomes and one containing inflorescences and pellets. Once this behavior was evident, PLS-DA was applied in order to reveal metabolites responsible for the segregation between different types of samples. Based on VIPs (Variable Importance Projection) obtained in the PLS-DA analyses, secondary metabolites were annotated (verified in house library and literature). Flavonoids and α- and β-acids were amongst the chemical classes annotated. These results revealed significant chemical distinctions between the samples, providing valuable insights into the composition of hops cultivated under tropical climate and chemical contribution of each structure analyzed, and further suggesting the method as a simple but robust strategy for hop chemical analysis.

Keywords: *Brazilian hops; glandular trichomes;metabolomics;LC-MS/MS.*