



Mass spectrometry strategies for the analysis of volatile plant secondary metabolite dynamics.

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The structural elucidation of increasingly small quantities of organic compounds is a routinely required task of the chemist, especially in natural product research laboratories. Among the analytical tools available, there is a wide variety of spectroscopic and spectrometric techniques. In plant systematics, the biological classification of plants, secondary metabolites have been used as taxonomic markers for nearly 200 years and targeted analysis of plants metabolites for various purposes dates back as far as the analysis of essential oils, performed since the introduction of gas chromatography (CG) in the early 1950's. The hyphenation of CG with mass spectrometry (MS) introduced a new perspective for ecological analysis and still an important research subject. In recent years, developments in these techniques have allowed the analyst to obtain valuable structural information of a given compound at low concentrations (at high sensitivity) and in an increasingly short time-period. Each analytical method provides different, complementary structural information about a given compound. When it comes to mass spectrometry (MS), it is possible to obtain data regarding the molecular weight and/or the molecular formula of compounds, the presence of heteroatoms, and the presence of functional groups, depending on the characteristics of the mass spectrometer. Tandem mass spectrometry (MS/MS) is also able to provide additional structural information through fragmentation of the compound of interest. Therefore, MS and MS/MS are powerful tools for the structural elucidation of a wide range of organic compounds. In this work we present a systematic investigation several volatile organic compounds (VOCs) from *Lychnophora* species (micro endemic Asteraceae specie restrict to "campus rupestris" from Brazilian "Cerrado") and the perspective for the use in metabolomic studies for ecological purposes combining different MS strategies.

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