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Plant metabolomics by MALDI-MS: Comprehension of ionization and fragmentation processes

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Abstract

By definition, metabolomics is the measurement of all the metabolites in a system (cell, tissue or organism). We developed a new method for metabolomic analyses of plants (Asteraceae) by MALDI-MS and proposed taxonomic classification the species using these metabolic fingerprints. The MALDI were selected due the sensibility, simplicity and ability to evaluate mixtures of substances. However, studies about the ionization of the secondary metabolites with different matrixes and the fragmentation pattern by LIFT method are necessary, so they were not reported yet. In positive and negative modes all series of fragment ions for *C*-flavonoids showed some the typical neutral losses, the same observed with ESI, from 90 and 120 u formed by a charge remote mechanism (moiety $^{0,3}X$ and $^{0,2}X$, respectively). In addition, for vicenin-2 the $^{0,3}X$ and $^{0,2}X$ pathway reactions were observed for both rings giving more confidence to the data. For apolar substances, they were only observed in the spectra when 2,4 lithium 2,5-dihydroxybenzoate was used as matrix, but the fragment ions were not observed for some classes. Therefore, in some cases the fragmentations of metabolites are different compared ESI data, the matrix can transfer different amounts of energy and inducing the fragmentation. For this reason, it was possible to detect fragment ions in the MALDI-MS analyses.

Biography

Denise Brentan da Silva has completed his Ph.D at the age of 26 years. She is currently a postdoctoral associate at Faculty of Pharmaceutical Sciences of Ribeirão Preto - University of São Paulo, working with MALDI analyses of secondary metabolites and imaging in tissues. She has published more than 16 papers in reputed journals, plus one book chapter.