

Dereplication of extracts from stems and leaves of *Metrodorea nigra* St. Hill (Rutaceae) by ESI-MS

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Abstract

Dereplication by ESI-MS of extracts from leaves and stems of a *Metrodorea nigra* (Rutaceae) specimen collected at the city of Rio de Janeiro, Brazil, showed that only one coumarin is also found among the ones previously identified from extracts of a specimen collected in São Paulo state, Brazil.

Introdução

Dereplication can be understood as a previous analysis by any methods which allow to identify compounds previously found in a mixture such as plant extracts, avoiding reisolation of these substances, if it is not the goal of the research. *Metrodorea nigra* (Rutaceae) is a plant species, commonly known as wild orange and a specimen collected in São Paulo, Brazil was chemically studied by Müller *et al.*¹ that isolated and identified several coumarins, alkaloids and dihydrochalcones from extracts of its fruits, leaves and stems. In order to compare chemical composition of the extracts from the samples of both São Paulo and Rio de Janeiro, there was performed a dereplication study, using ESI-MS (Eletronspray Ionization-Mass Spectrometry). ESI-MS is a technique quite useful to obtain both molecular weights and fragmentation patterns, in positive or negative mode, of organic compounds such as secondary metabolites². Data obtained might be able to explain variation in the chemical composition of the extracts from specimens cultivated in different geographic regions.

Resultados e Discussão

Leaves and stems of a *M. nigra* specimen were collected in the Botanical Garden of Rio de Janeiro, Rio de Janeiro, Brazil. Ethanol extracts were prepared by percolation from this dry-grinded material. Samples of both extracts were solubilized in methanol/water (9: 1) and analyzed by ESI-MS through direct infusion into an Amazon SL spectrometry (ESI-IT), electrospray ionization in the 39ª Reunião Anual da Sociedade Brasileira de Química: Criar e Empreender

positive and negative modes, using as mass detection a range between 0 and 900 amu. M/z values of the peaks in the ESI-MS spectra (positive and negative modes) were compared with the molecular weight of the previously identified metabolites¹ and it was found that only deoxybruceol coumarin (Figure 1) is present in both extracts at high relative amounts.

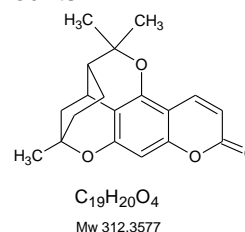


Figure 1. Coumarin deoxybruceol

This result was achieved by comparing molecular weight of deoxybruceol (312.3577) with the peak observed at 311.1706 (M-H⁺), demonstrating a 99.94% similarity. Structure was confirmed by analysis of its fragmentation pattern at the MS spectra. Other peaks at m/z 283.2645, m/z 325.1851 m/z 339.2073 might be related to other coumarins or dehydrochalcones different from the ones previously found.

Conclusões

Results of the ESI-MS analysis suggest a variation at the chemical composition of extracts from leaves and stems of *M. nigra* in specimens collected in two different states of Brazil.

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¹Müller, A. H.; Vieira, P. C.; Da Silva, M. F. das G. F.; Fernandes, J. B. *Phytochemistry*. **1995**, *40* (6), 1797.

²Smith, W. F.; Smyth, T. J. P.; Ramachandran, V. N.; O'Donnell, F. e Brooks, P. *Trends in Analytical Chemistry*. **2012**, *33*, 48.