

Definition of gas-phase fragmentation reactions of spirocyclic alkaloid by electrospray ionization tandem mass spectrometry: Applications in metabolomics studies

Thais Guaratini, Norberto Peporine Lopes, Denise Brentan da Silva and João Luis Callegari Lopes
University of São Paulo, Brazil

The genus *Erythrina* (Fabaceae) comprises approximately 115 species distributed in all tropical and subtropical Forests. Erithrinic alkaloids present tranquilizer, anxiolytic, sedative effects. There is a great interest in the development of new medicines for central nervous disorders from erithrinic alkaloids. In this way, investigations of possible sources of alkaloids have revealed a sample with almost 80% of erythralin as the major alkaloid and these materials are under pre-clinical studies. An important step for the development of oral medicines is the definition of possible metabolites in gut microbiota and internal phase 1 and phases 2 reactions. Electrospray ionization mass spectrometry has been shown to be a good choice technique to identify these products. The understanding of the mechanism involved in each fragmentation reaction is now helping to define the gas phase chemical reactions after the collisional activation and comparative analysis of different energy transfers can corroborate to obtained data. Systematic ESI-MS/MS and ESI-MSⁿ analysis of the spirocyclic alkaloid erythralin showed an expected H₂ neutral elimination reaction. We have investigated the formation of these ions by accurate-mass electrospray tandem mass spectrometry with different analyzers and the data suggests a possible unimolecular reaction involving metastable ions. Metastable ions are very rare ions and all these fragmentation pathways are not observed in quadrupole analyzers. Based on this observation a complete fragmentation map was defined and applied for metabolomic studies of phase one reactions. Besides, a new metabolite was detected and the structure defined by the fragmentation maps.

Biography

Thais Guaratini has completed his Ph.D. at the age of 29 years from University of São Paulo. She is currently a postdoctoral associate at Chemistry Department, USP, studying kinetic disposition of natural products constituents and especially the oxidative metabolism of phase 1. She has worked as a visiting researcher at IACR-Harpenden, UK, University of Bristol, UK for the doctorate and the laboratory of cell biology at Heinrich-Heine University, Germany. She has published 17 papers in reputed journals, plus 4 awards, 6 book chapters and publishing a book.

thais@lychnoflora.com.br