

Natural Products and Synthetics

Mass Spectrometry in Microbial Metabolomic Analysis

Eduardo José Crevelin^{1*}, Jussara Batista da Costa¹, Itamar Soares de Melo², Luiz Alberto Beraldo de Moraes¹

***ejcrevelin@pg.ffclrp.usp.br**

¹ University of São Paulo – Department of Chemistry - FFCLRP

² Laboratory of Environmental Microbiology - Embrapa/Jaguaríuna

Metabolomics aims at the comprehensive and quantitative analysis of wide arrays of metabolites in biological samples¹. Currently, two complementary approaches are used for metabolomic investigations: metabolic profiling and metabolic fingerprinting. Metabolic profiling focuses on the analysis of a group of metabolites either related to a specific metabolic pathway or a class of compounds. Usually, metabolites are selected for analysis and specific analytical methods are developed for their determination.

The application of MS for analysis of secondary metabolites has grown dramatically over the last two decades, and today MS is the single most important detector method in biotechnology. MS plays an important role in the chemical analysis of metabolites mainly because of its accessibility, versatility, and powerful technology that are best-suited to solve research and analytical problems in the metabolome field².

Thus, the aim of this study was to analyze metabolite profiles of organic crude extracts obtained from actinomycetes in different cultivation medium by direct-infusion MS.

The results showed that there are differences in the production of secondary metabolites occurred in response to the growth conditions. The dereplication strategy for the analysis of the secondary metabolites has been developed. First, full scan total ion chromatogram (TIC), scanning m/z 100-1200, was acquired in both positive and negative modes. Ionization of compounds was better in positive mode. Thus, the dereplication was carried out in the mass range of m/z 750-850. Therefore, the data suggest that the secondary metabolites located in this mass range may belong to class of polyketide compounds.

[1] Dettmer, K.; Aronov, P.A.; Hammock, B.D. *Mass. Spectrom. Rev.* **2007**, 26, 51-78.

[2] Villas-Bôas, S.G.; Mas, S.; Akesson, M.; Smedsgaard, J.; Nielsen, J. *Mass. Spectrom. Rev.* **2005**, 24, 613-646.