Two-Dimensional Tandem Mass Spectrometry as a Method for Bacterial Profiling

Lucas Szalwinski, L. Edwin Gonzalez, Thomas Sams, Eric Dziekonski, Graham Cooks Department of Chemistry, Purdue University, West Lafayette, Indiana, 47907, United States

A modified quadrupole ion trap mass spectrometer was used to positively identify sporulated bacteria using a two-dimensional tandem mass spectrometry (2D MS/MS) data domain. Bacillus subtilis and Bacillus thuringiensis were split into a vegetative and sporulation group where they were both subjected to microwave radiation for the purpose of de-sporulation. The characteristic lipid profiles were observed in both the vegetative and sporulated states while the metabolomic profile clearly differentiated the two. This identification was performed in a 1.2 second negative scan using nanoelectrospray ionization. The 2D MS/MS spectrum allowed for the immediate structural identification of phosphatidylglycerol (PG) fatty acid losses along the product scan lines. The presence of 2,6- pyrdinedicarboxylic acid, dipicolinic acid (DPA) was clearly distinguishable from the metabolite background. This experiment shows that 2D MS/MS is a technique that can provide easily identifiable and rapid structural information over a wide range of analytes.