Rapid detection of pathogenic bacteria using secondary electrospray ionization-mass spectrometry (SESI-MS)

In this work, we applied secondary electrospray ionization-mass spectrometry (SESI-MS) to detect and characterize the VOCs produced by strains of *Pseudomonas aeruginosa, Staphylococcus aureus, Escherichia coli,* and *Salmonella typhimurium* (i.e., Gram positive and negative species). The metabolic profiles from the headspace of bacterial cultures were characterized by SESI-MS. Representative spectra of each species were obtained under the same growth condition (24 h; aerobic; 37°C; TSB). Thirteen compounds were identified or tentatively identified from the headspace of these bacterial cultures and the combination of these VOCs created a unique pattern for each species. Several compounds such as, ethanol, acetone, and acetic acid, are produced through central metabolic pathways, and are therefore commonly observed for many species of bacteria, and in human breath. The majority of these compounds were observed in the mass spectra at m/z = M+1. However, a few compounds, such as butanol and isopentanol, were observed at a mass of M-17, indicating the loss of a water molecule during sample analysis, which is a common occurrence for primary alcohols. Some of the compounds that are present in the headspace of these bacteria give rise to more than one peak in the mass spectrum, either due to dimer formation (m/z = 2M+1) or fragmentation during ionization. Meanwhile, we have used principal component analysis (PCA), without any peak identification information, to demonstrate the ability to discriminate species by their volatile profile. The first three components (54.34%, 17.17%, and 11.21% variability, respectively) exhibited a clear separation between the volatile metabolic profiles of each species. To the best of our knowledge, this is the first time that SESI-MS has been used to characterize bacterial VOCs, and our data confirm the utility of this technology in real-time identification of bacterial species.