

ATMOSPHERIC PRESSURE GAS CHROMATOGRAPHY-MASS SPECTROMETRIC PROFILING OF VOCs IN FRUITS

Manoj S. Ghaste^{1,2}, Vladimir Shulaev^{1,2}, Fulvio Mattivi¹

¹ Food Quality and Nutrition Department - Edmund Mach Foundation, Research and Innovation Centre, Via E. Mach 1, 38010 San Michele a/A, Italy

² Department of Biological Sciences - University of North Texas, 305220, TX 76203-5017 Denton, United States

Gas chromatography coupled with mass spectrometry (GCMS) is a well-established analytical approach for volatile compounds analysis and metabolomics. The most widely used ionization technique in GCMS is electron ionization (EI), which produces library searchable spectra dominated by fragments. The molecular ion in EI spectrum is often of very low abundance or absent. Many plant terpenoids have same molecular formula and shows matching fragmentation pattern when using EI, therefore any minor dissimilarity in the relative abundances of the masses in a spectrum lead to a false search result in NIST. Also lack of molecular ion information can give incorrect compound identification, if using spectral matching alone. Alternative approaches, such as the chemical ionization (CI), can be optimized to provide a molecular ion with reduced fragmentation, but with the serious drawback of a major loss of the sensitivity.

Atmospheric pressure gas chromatography coupled with mass spectrometry (APGC-MS) is an ionization technique that generates a spectrum conserving the molecular ion species with minimal fragmentation; additionally the system offers high mass accuracy, which is extremely useful in structure elucidation of unknown volatiles. We are establishing an analytical method employing APGC-MS for VOCs in fruits like Grape and Strawberry. In first phase we have done optimization of instrumental parameters using mixture of pure reference standards of fruit aroma compounds, this also aided in understanding ionization patterns of VOCs using APGC-MS since there is no database (like NIST MS) is available for primary identification of the compounds. Using injections of pure reference standards we started developing in-house APGC-MS library of the fruit VOCs. Parallely, efficiency of thermal desorption system (TDS) for the extraction of VOCs also has been tested.