

EPA Ion Composition Elucidation (ICE): a High Resolution Mass Spectrometric Technique for Identifying Compounds in Complex Mixtures

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Abstract

When tentatively identifying compounds in complex mixtures using mass spectral libraries, multiple matches or no plausible matches due to a high level of chemical noise or interferences can occur. Worse yet, most analytes are not in the libraries. In each case, Ion Composition Elucidation (ICE) provides a means for identifying compounds. This poster illustrates an example of each problem and its solution.

Ion Composition Elucidation (ICE) to Provide Additional Mass Spectral Data

ICE was developed by the Environmental Chemistry Branch of the National Exposure Research Laboratory of the Office of Research and Development of the U.S. Environmental Protection Agency to help identify compounds in environmental samples. ICE has two facets, data acquisition using Mass Peak Profiling from Selected Ion Recording Data (MPPSIRD) and automated data interpretation using a Profile Generation Model (PGM).^[3]

Three Compound Identification Problems

1. Multiple Plausible Library Matches

The mass spectrum in Figure 1a is a background-subtracted mass spectrum for a compound in an extract of 12 L of effluent from a tertiary waste water treatment plant. Figures 1b-g are NIST library matches over the same mass range. The isomers in parenthesis in Figure 1 also had similar NIST mass spectra. The compound that provided the mass spectrum was present in the extract at an ultra-trace level. Chemical noise, coelution of compounds in the complex extract, and septum and column bleed components generally result in background-subtracted mass spectra containing extraneous ions or lacking low-abundance ions expected from the analyte. Hence, none of the NIST library matches can be ruled out without additional data.

