

RAPID ANALYSIS THROUGH NEW ADVANCES IN GC-TOFMS TECHNOLOGY

GLEN STUTCHBURY^a, RITCHARD PARRY^b, MARTIN SCHAUT^a AND ROSS GIORDANO^a^a LECO Australia Pty. Ltd. 4/10 Salisbury Road, Castle Hill, NSW 2154 Australia^b LECO Corporation, 3000 Lakeview Avenue, St. Joseph, MI 49085

The combination of fast chromatography techniques with mass spectrometer detectors has been plagued by the slow acquisition rates of scanning mass spectrometers. The narrow chromatographic peaks generated by these fast GC techniques range anywhere from 50 ms to 1 second wide at the base and cannot be adequately defined with spectral acquisition rates of only 1 to 10 spectra/second. Time-of-flight mass spectrometers have always had the potential for rapid data collection but only recently has high speed electronics advanced to a point where that potential can be realized. A unique TOF system design capable of acquiring up to 500 mass spectra/second across a range from 5u to 1000u will be presented and discussed.

A common result from attempts to reduce chromatographic separation time is the loss of chromatographic resolution. Coeluting peaks can be quite tedious to locate and identify. In many cases the time saved by reducing the separation time is quickly cancelled by the longer time spent processing data from coelutions. The unique spectral continuity and reproducibility found in TOF data can be used to develop software solutions for these data processing problems. Sophisticated peak location algorithms can be developed to indicate the presence of low concentration analytes indiscernible in the Total Ion Chromatogram as well as to indicate the presence of multiple components in a coelution (see Figure 1). Once the peak locations are identified in a coelution, the spectral continuity of TOF data can be used to develop additional algorithms to deconvolute the overlapping mass spectra. The application of these algorithms in the analysis of a variety of sample types such as petroleum fuels, flavors, fragrances, food products, and beverages will be presented and discussed.

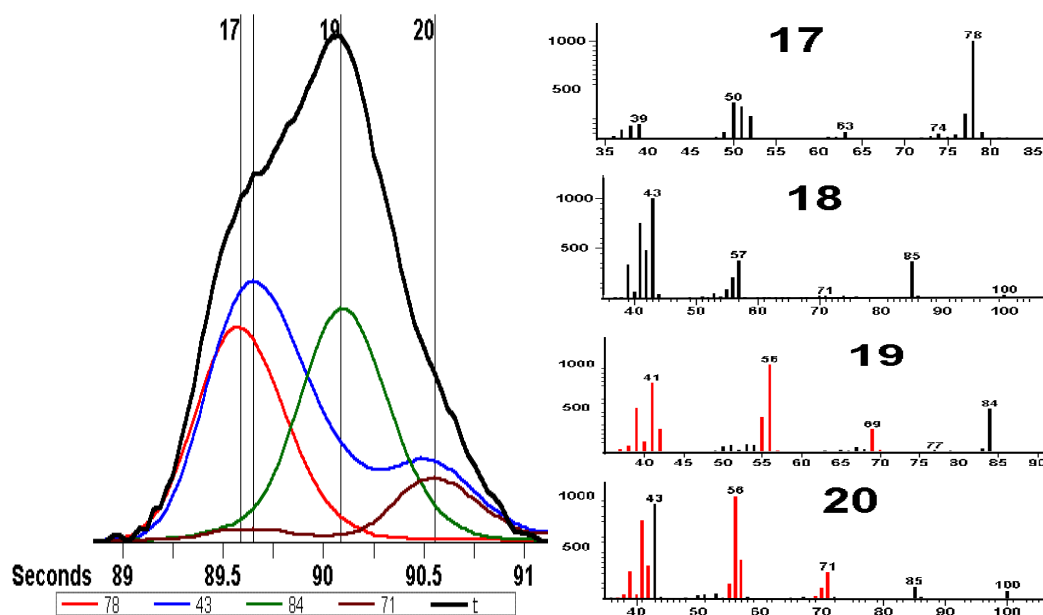


Figure 1: Left – A Peak Location algorithm indicates the positions of four analytes in a coelution within a mixture of Naphtha Hydrocarbons.

Right – A Deconvolution algorithm accurately deconvolutes the mass spectra from the four coeluting analytes.

Peak 17 – Identified as Benzene by NIST library search (Similarity of 888)

Peak 18 – Identified as 2-Methylhexane by NIST library search (Similarity of 863)

Peak 19 – Identified as Cyclohexane by NIST library search (Similarity of 924)

Peak 20 – Identified as 2,3-Dimethylpentane by NIST library search (Similarity of 901)