Pegasus®

Acquisition Rate for Peak Find and Deconvolution

In gas chromatography (GC) coelutions occur when samples are complex, or when the chromatography is compressed to make sample analysis faster. To ease the burden of data processing under these conditions, automatic Peak Find and Spectral Deconvolution routines are part of the LECO ChromaTOF™ software platform. These algorithms are made possible by Time-of-Flight Mass Spectrometry (TOFMS)—specifically, acquisition rates up to hundreds of spectra/second and unskewed mass spectra. Neither of these TOFMS features is available with scanning mass spectrometers, such as quadrupoles or magnetic sectors. To demonstrate the power of TOFMS for Peak Find and Spectral Deconvolution, two compounds were made to coelute under fast GC conditions, while acquiring spectra at various acquisition rates with a LECO Pegasus Gas Chromatograph—Time-of-Flight Mass Spectrometer.

Materials and Methods

Gas Chromatography

Retention Gap:	5 m x 0.53 mm Siltek-deactivated guard column (Restek)
Column:	10 m x 0.32 mm x 0.91 µm Rtx-TNT (Restek)
Carrier:	Helium at 5 ml/min, constant flow
Injection:	1 µl on-column at 85°C (tracks 5° above GC oven)
Oven Program:	80°C (0.5 min) to 260° at 55°/min

Mass Spectrometry

Ionization:	Electron ionization at 70eV
Source Temperature:	180°C
Stored Mass Range:	45 to 350 u
Acquisition Rate:	10, 20, 30, or 40 spectra/sec.
Total Run Time:	3.77 min

Results

Figure 1 shows extracted ion chromatograms where 2-methyl-4-nitroaniline and 2,4,6-trinitrotoluene (TNT) coelute. The TOFMS acquisition rate was 40 spectra/second. The two vertical lines marking the peak apexes represent the two peaks located by ChromaTOF Peak Find. At rates of 10, 20, and 30 spectra/second, only one peak was located, resulting in the coeluted mass spectrum shown in Figure 2. This is not surprising considering that the peak apexes for these compounds are only 175 ms apart.

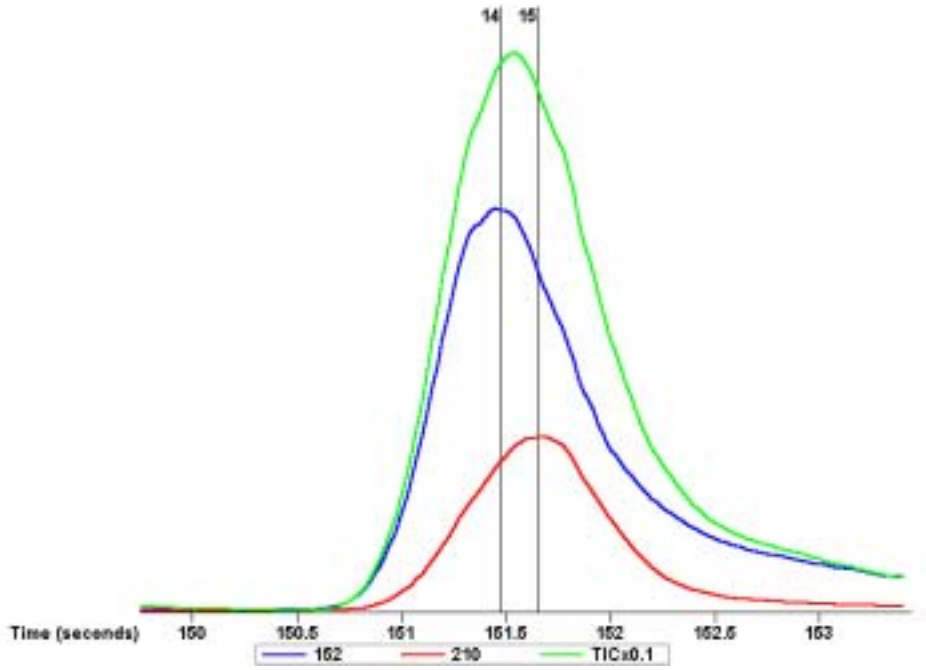


Figure 1. *Automatic Peak Find of 2-methyl-4-nitroaniline (152) and TNT (210) using a 40 spectra/second TOFMS acquisition rate. The peak apexes are only 175 ms apart. Vertical lines (14 and 15) represent peaks located automatically by ChromaTOF. The green TIC plot, reduced to stay on scale, indicates the coelution problem.*

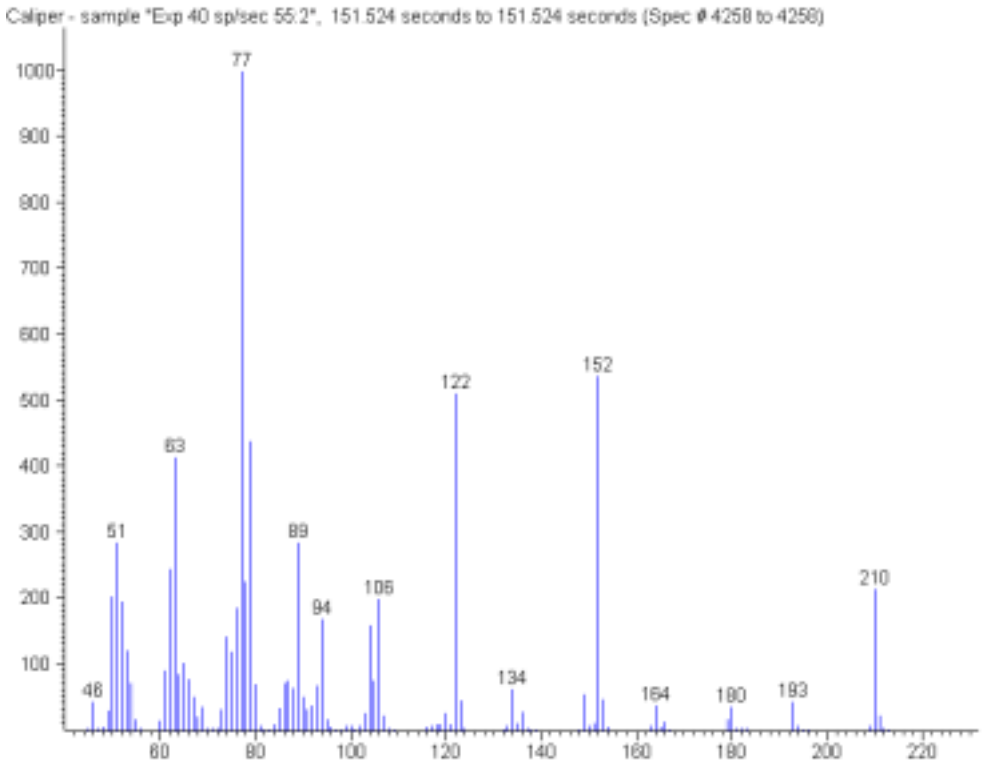
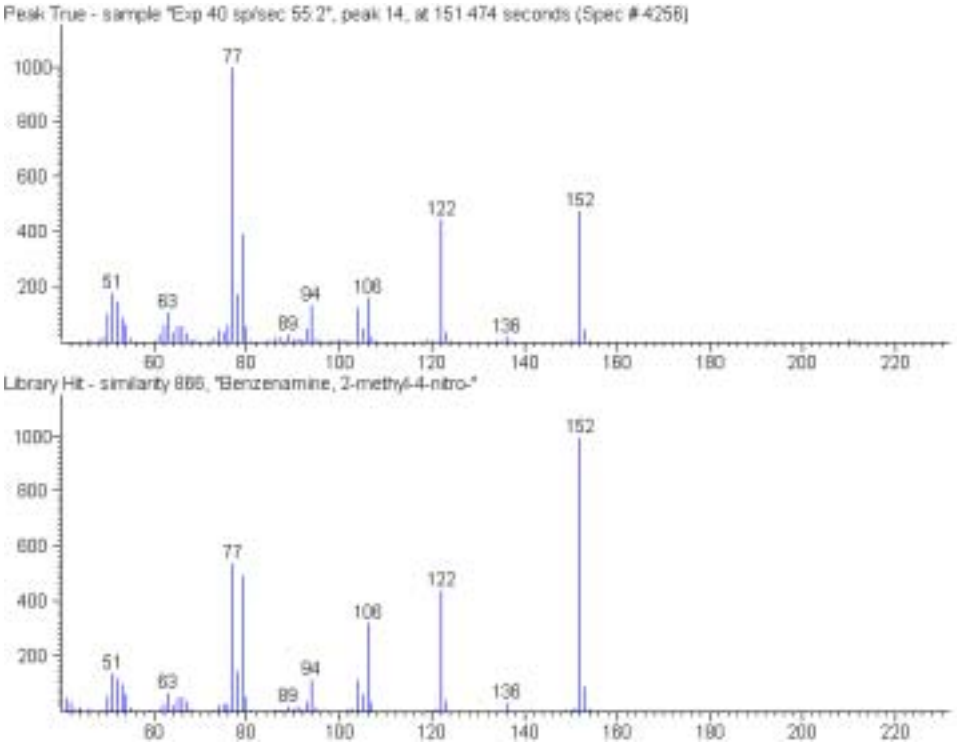


Figure 2. *Coeluted mass spectrum of 2-methyl-4-nitroaniline and TNT when only one peak was located due to insufficient acquisition rate. The 77, 122, and 152 ions are from the 2-methyl-4-nitroaniline, and the 63, 89, and 210 ions are from TNT.*

Figures 3 and 4 display the deconvoluted mass spectra for 2-methyl-4-nitroaniline and TNT, versus the NIST library mass spectra for these same compounds. The library matches for each spectrum



are excellent.

Figure 3. *Deconvoluted (top) and NIST library (bottom) mass spectra for 2-methyl-4-nitroaniline.*

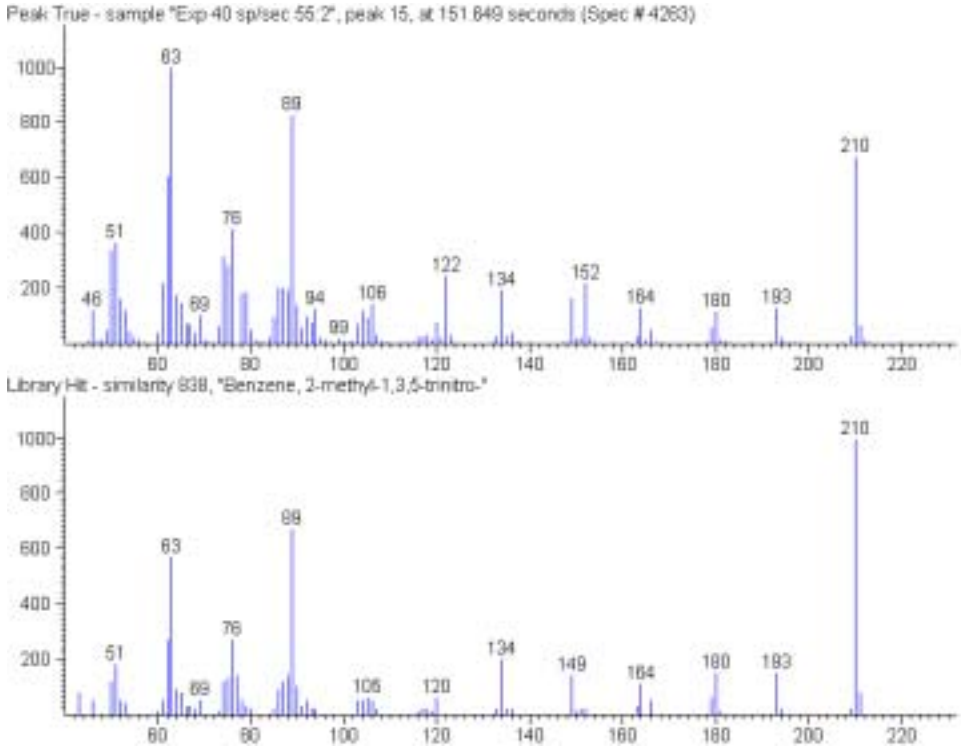


Figure 4. *Deconvoluted (top) and NIST library (bottom) mass spectra for TNT.*

Conclusion

The fast acquisition rates and spectral reproducibility of TOFMS are necessary to support Peak Find and Deconvolution routines. These functions are not available with magnetic sector or quadrupole mass spectrometers.

LECO Corporation **• 3000 Lakeview Ave. • St. Joseph, MI 49085-2396**
Phone: 800-292-6141 • Fax: 269-982-8977 • info@leco.com • www.leco.com