Pegasus® HT-C and Pegasus 4D-C

Leco®
Delivering the Right Results

What is missing in your sample? Is it important?

The *Pegasus* 4D GCxGC-TOFMS from LECO is trusted by scientists around the world, working in diverse markets and industries, who are all looking for answers to these questions.

By combining LECO's pioneering GCxGC technology with the speed and sensitivity of the *Pegasus* HT GC-TOFMS, the *Pegasus* 4D makes it easy to see what's hidden in your sample. A second dimension of chromatography separates coelution very clearly for more complete sample analysis.

ChromaTOF

For complete patent information, see specification sheet.

What's New *PEGASUS* HT-C and 4D-C

- The same great reliability and performance in a new and updated package
- All new modernized electronics and hardware allow for unprecedented data acquisition and GCxGC control
- New design meets RoHS compliance standards for the European market
- Identical performance to the previous generation
  - Same ion optical elements yield excellent TOF performance
  - Same ion source design leads to the established low-maintenance profile
  - Same easy-to-use, well-known ChromaTOF® brand software with features optimized for efficiency and instrument operation

Diagram of GCxGC/GC-TOFMS Instrument

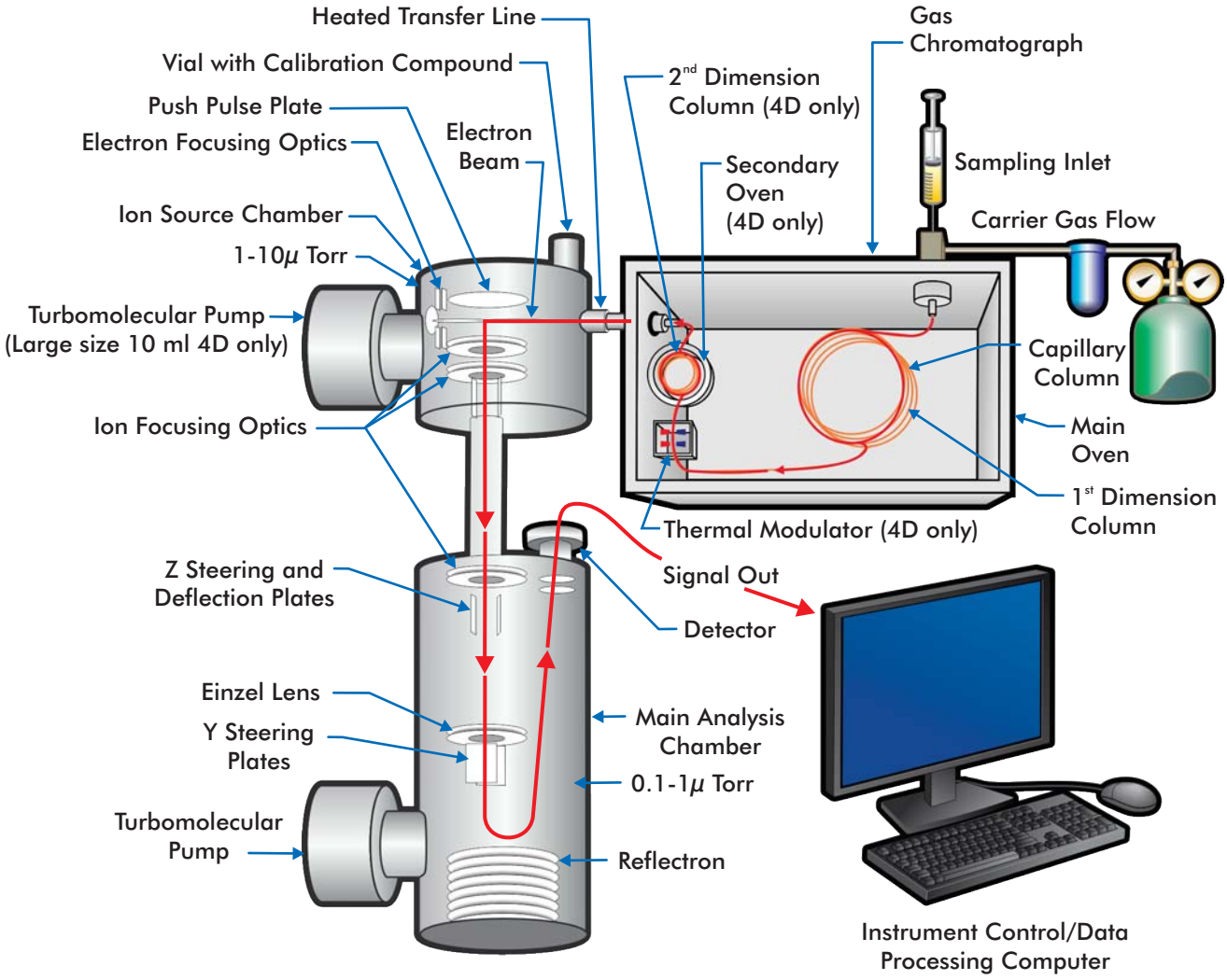

Figure 1. The entire modulator is mounted inside the primary GC oven. Control of the GC autosampler, GC, LECO's GCxGC thermal modulator, and the Pegasus TOFMS is fully integrated within ChromaTOF.

Complex Sample Analysis

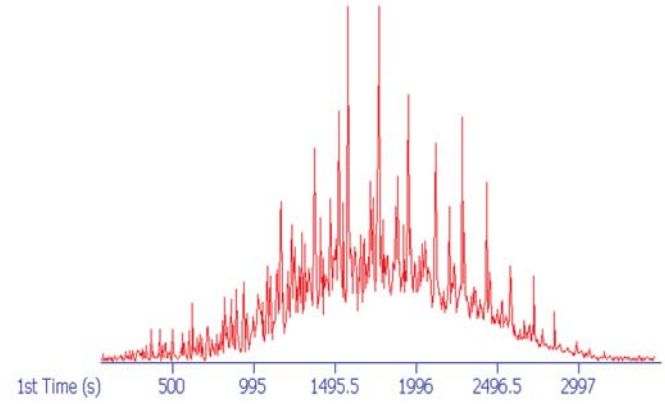

Figure 2. Traditional GCMS analysis of petroleum (678 analytes detected).

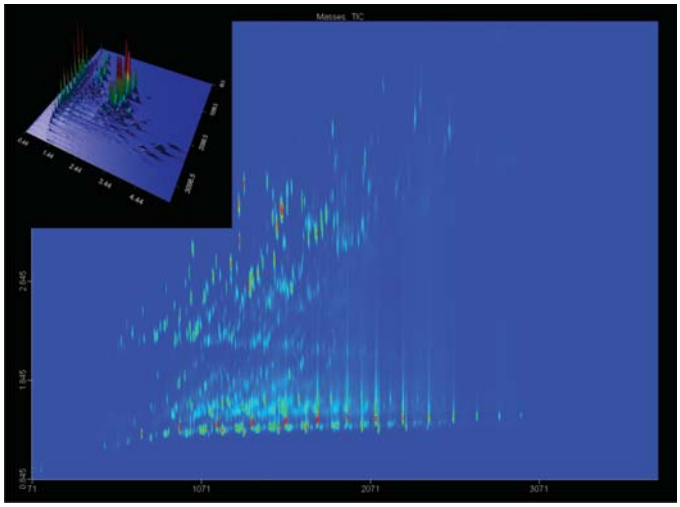

Figure 3. GCxGC-TOFMS analysis of petroleum (1,246 analytes detected).

The GCxGC Advantage

The demands of complex samples (such as the petroleum sample shown in Figure 2) quickly overwhelm traditional GCMS analysis techniques. Coelution is the problem.

LECO provides a solution for complex sample analysis with the *Pegasus* 4D, the pre-eminent MS detector for Comprehensive Two-Dimensional GC (GCxGC). The High-Definition sample resolving capabilities of the *Pegasus* 4D and the data processing features of *ChromaTOF* offer every laboratory the ability to characterize and quantify even the most challenging samples.

Figures 2 and 3 are petroleum samples analyzed by both GC-TOFMS and GCxGC-TOFMS. Figure 2 clearly shows the complexity of the sample. Without the resolving capabilities of the *Pegasus* 4D, accurate characterization of the mixture would be impossible (Figure 3).

- Spectral collection rates up to 500 full-range mass spectra/second (500 Hz)—the *Pegasus* is the only MS detector capable of true comprehensive multi-dimensional chromatography
- Cryo-focusing prior to release on the secondary column provides up to a tenfold increase in analyte detectability
- True Signal Deconvolution®—no other MS manufacturer in the world can match LECO's deconvolution experience and success
- Automated Peak Find
- Wide dynamic range (4 orders of magnitude)
- Maintenance-free ion source (no cleaning required)
- A robust quad-jet, dual-stage thermal modulator
- Optional consumable-free thermal modulator
- Secondary oven for enhanced selectivity

Variable Modulation

An essential principle of GCxGC research states that the use of the shortest possible modulation period maximizes chromatographic resolution in the first dimension. Historically, this has meant chemists have had to employ a modulation period identified by the latest eluting analyte in the 2nd dimension. Now available with *ChromaTOF,* variable modulation allows chemists to incrementally increase the modulation period only as needed. This revolutionizing capability allows for the incredible separations of complex mixtures expected from the leaders in GCxGC technology.

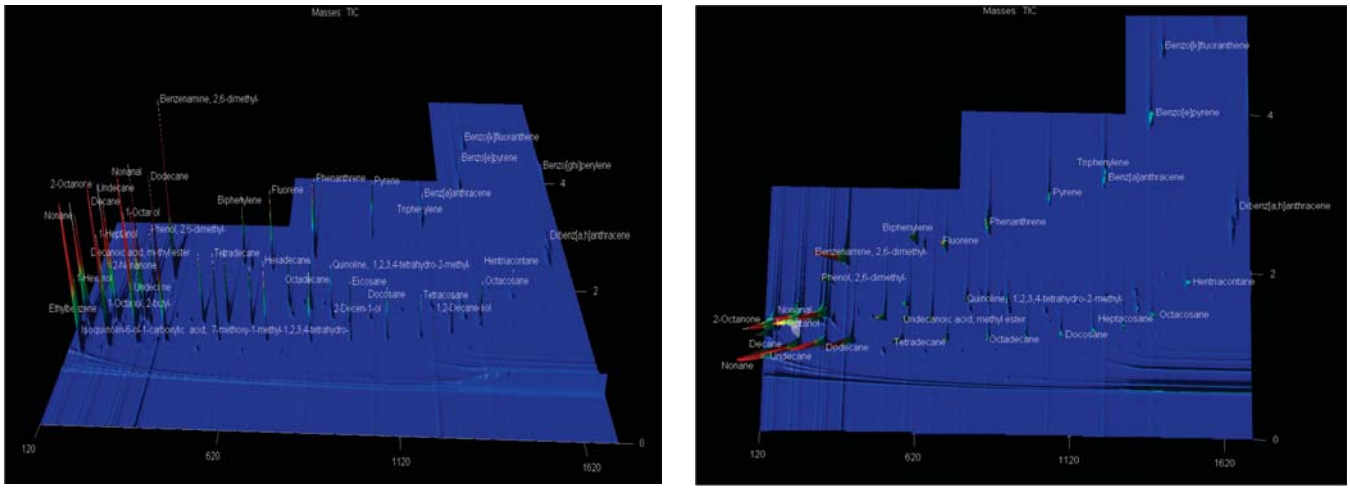

Figure 4. Contour plots of a single test mixture displaying the use of variable modulation from multiple views.

The Power of Time-of-Flight Mass Spectrometry

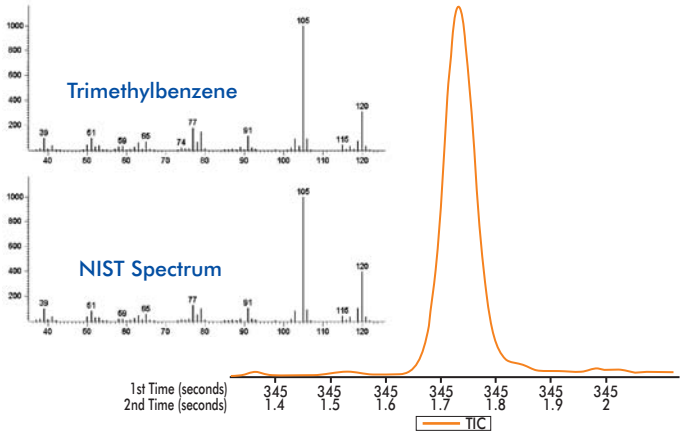

Figure 5. The 150 millisecond-wide trimethylbenzene GCxGC peak is easily defined and identified at a mass spectral acquisition of 200 spectra/second.

TOFMS—What Else Is In Your Sample?

As part of the cryo-focusing process in the GCxGC modulator, analyte bands that elute from the first column are significantly sharpened prior to being released into the second column. As a result, peaks ranging from 50 to 200 milliseconds wide are produced (Figure 5). These narrow peak widths require a detection system that is capable of collecting data at rates of 100 Hz or more in order to adequately characterize the shape of the chromatographic peak.

Only the *Pegasus* TOFMS, with continuous full-range mass spectral acquisition rates at up to 500 Hz, offers MS data with sufficient data density to address the requirements of any GCxGC separation. Spectral quality at these high acquisition rates is maintained in the *Pegasus* TOFMS as seen in Figure 5.

Qualitative Benefits of TOFMS

The power of the *Pegasus* TOFMS can also be seen in the qualitative benefits that GCxGC provides. By nature of the orthogonal separation system used in GCxGC, very structured chromatograms are produced showing distinct bands of analytes grouped by specific chemical characteristics (Figure 6). Using these chemical characteristics as a guide, more accurate individual analyte identification can be obtained from the *Pegasus* TOFMS.

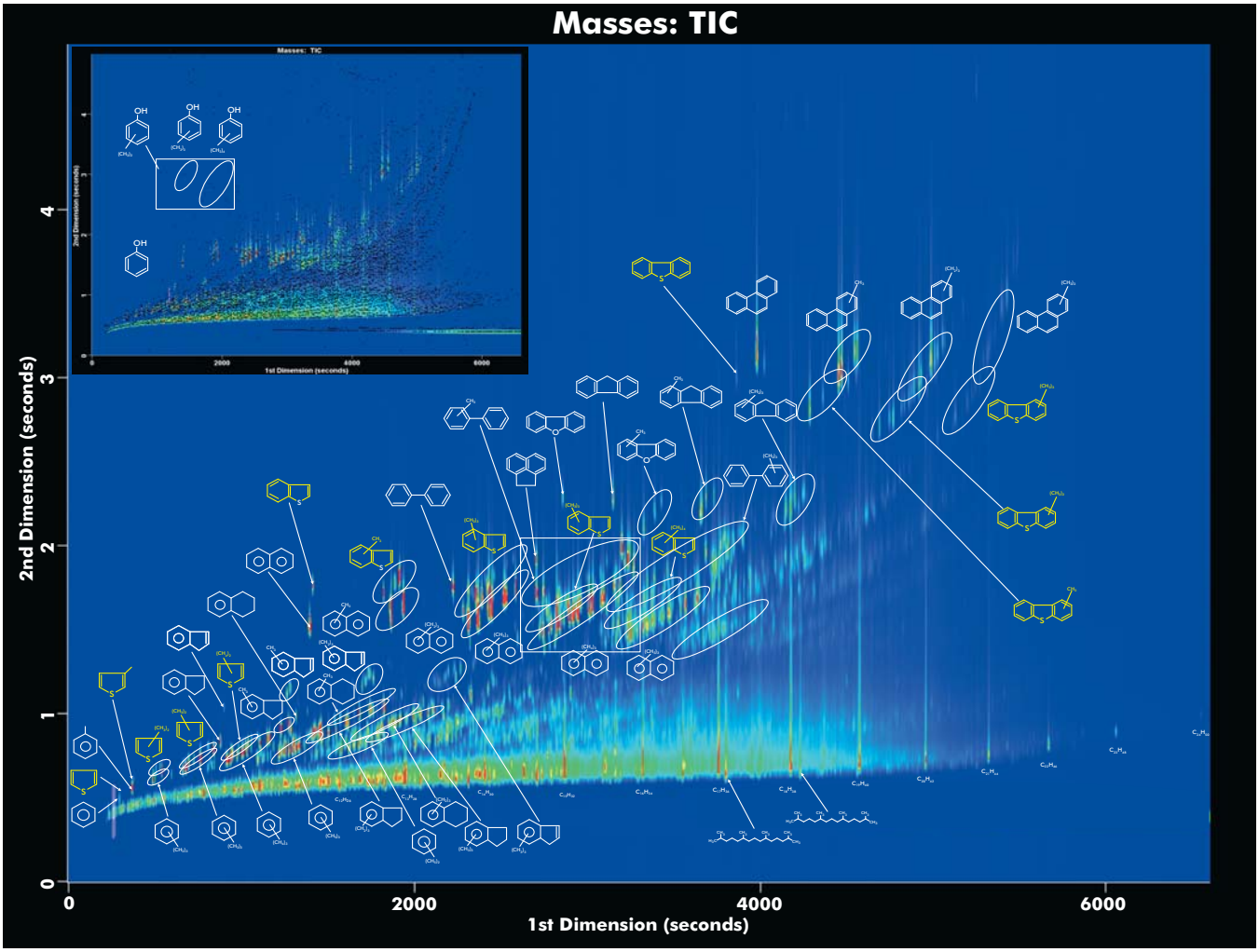

Figure 6. Complex sample characterization of diesel fuel is significantly simplified due to the structured GCxGC chromatogram that produces distinct bands for analyte chemical classes and the specific analyte identification provided by the TOFMS.

ChromaTOF Features

Automated GC and GCxGC Peak Finding

In addition to offering fully integrated system control from a single computer and software package, *ChromaTOF* provides fully automated processing of GC and GCxGC-TOFMS data. From easily prepared Data Processing Methods, a complete sample assay can be obtained—including qualitative characterization of the sample and quantitative data for specific analytes of interest.

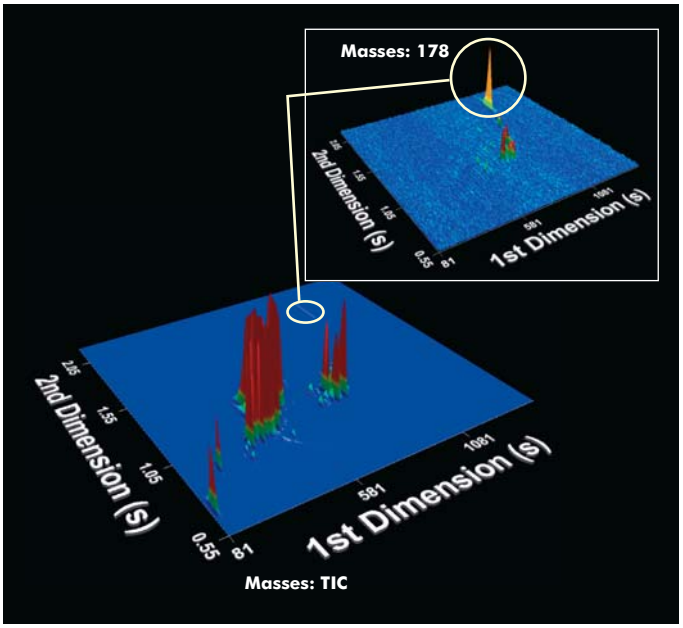

Figure 7. TIC surface plot for lime oil shows no peak in the gray highlighted region, however, viewing unique mass 178 the presence of a trace level compound is observed. In order to find the Citrapene peak, you must be able to look beneath the baseline—only ChromaTOF can deliver this to you automatically.

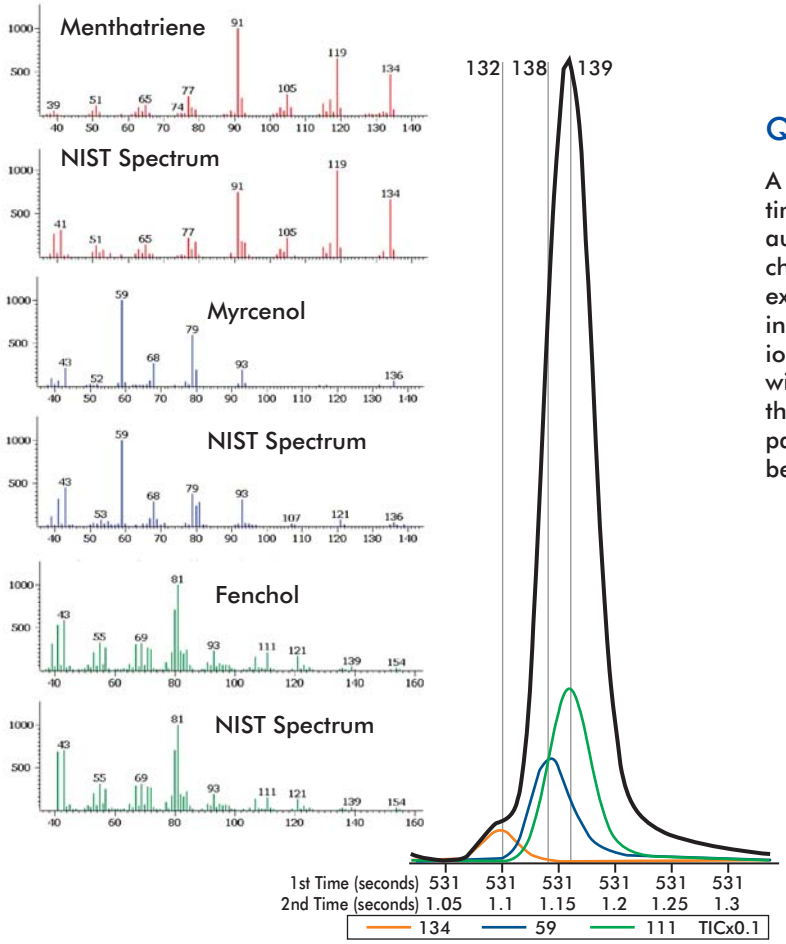

Figure 8. Automated Peak Find of three coeluting analytes in a 0.3 second portion of a second-dimension chromatogram.

Qualitative Sample Characterization

A good software package reduces the amount of time it takes to decode your analyses. *ChromaTOF* automatically finds all peaks throughout the entire chromatogram and deconvolutes them in order to extract a clean mass spectrum. These peaks include those that are hidden beneath the total ion chromatogram (TIC) and those that coelute with other compounds in the sample. Compare that to the manual requirements of other software packages and the advantage of *ChromaTOF* becomes undeniable.

- Automated Peak Finding
- True Signal Deconvolution to produce extracted mass spectra free of interfering signal
- Statistical Compare feature provides peak alignment and Fisher Ratios; data can be easily exported and analyzed by peripheral software for generating PCA plots

Automated Quantitative GC and GCxGC Analysis

ChromaTOF offers fully automated quantitative analysis for use with GC- and GCxGC-TOFMS data.

- Unlimited number of Calibration Points
- Unlimited number of Internal Standards
- Multi-order calibration curves
- Individual point weighting factors
- Extended Range Calibrations
- Retention Index Probes
- Ion Ratios

A variety of electronic reporting and exporting functions are available for distribution of the quantified results.

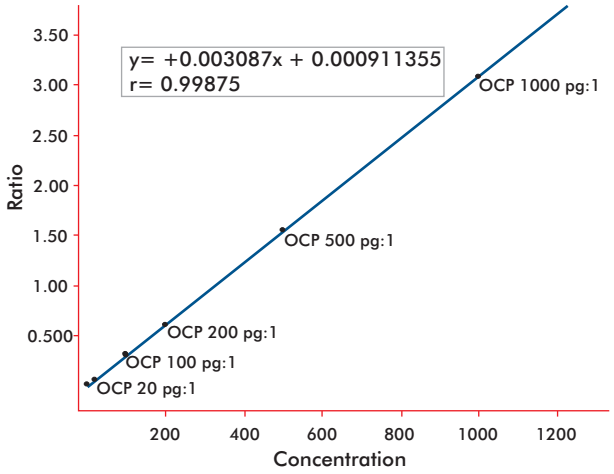

Figure 9. 4,4′-DDE calibration curve from 0.2 pg/µL to 1000 pg/µL.

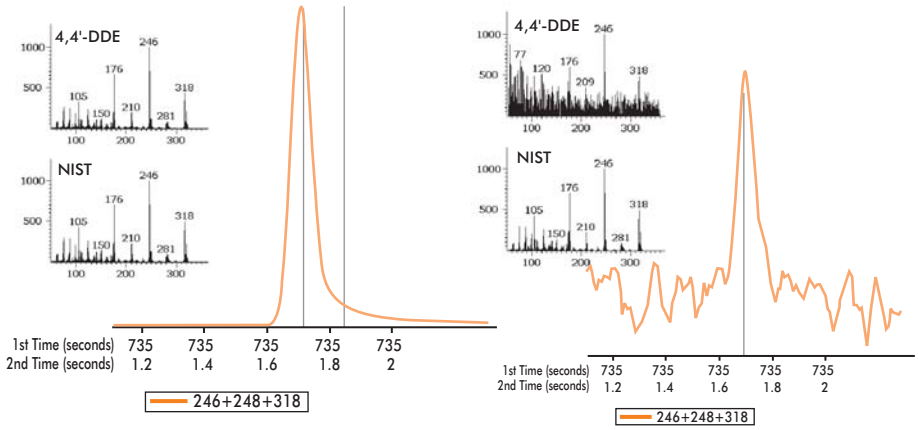

Figure 10. 1000 pg (left) and 0.2 pg (right) 4,4′-DDE Standards.

Analyte Calibration

Figure 9 depicts a GC and GCxGC-TOFMS calibration curve for the organochlorine pesticide degradate 4,4′-DDE. The calibration ranges from 0.2 pg to 1000 pg on column to address the requirements for pesticide analysis in food matrices. The high and low level 246u extracted ion profiles are displayed, along with the mass spectrum for the 0.2 pg/µL and 1000 pg/µL standards in Figure 10.

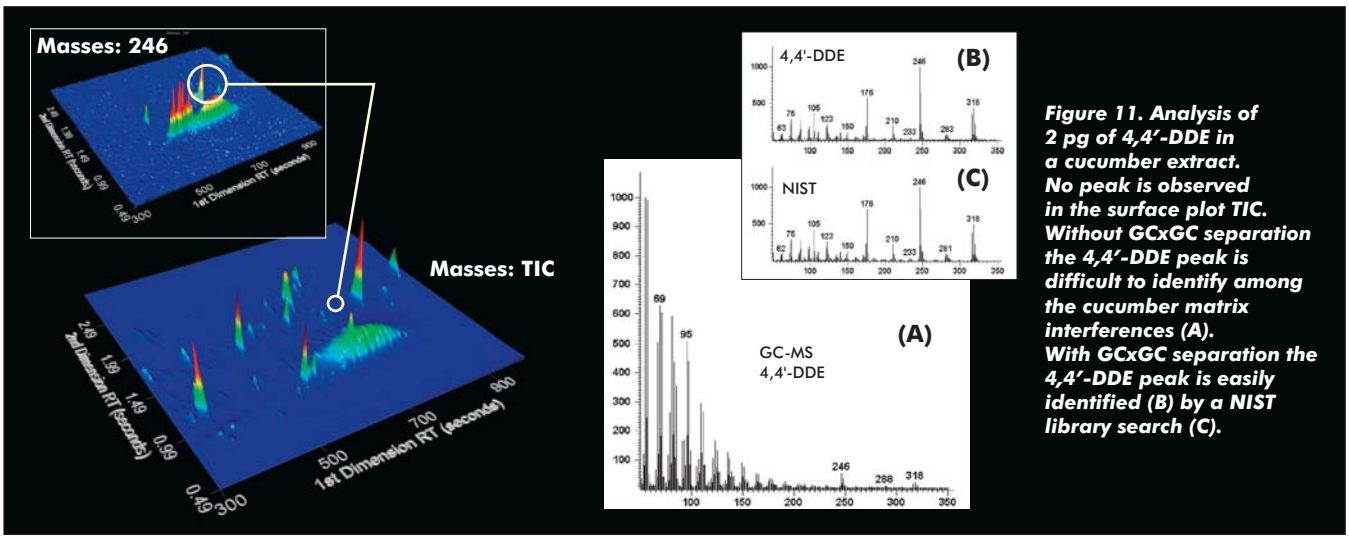

Figure 11. Analysis of 2 pg of 4,4′-DDE in a cucumber extract. No peak is observed in the surface plot TIC. Without GCxGC separation the 4,4′-DDE peak is difficult to identify among the cucumber matrix interferences (A). With GCxGC separation the 4,4′-DDE peak is easily identified (B) by a NIST library search (C).

Sample Quantification

Trace level quantification is frequently complicated by matrix interference. In Figure 11, the matrix components of a cucumber extract are clearly displayed in the surface plot. The added resolving power of GCxGC and GC-TOFMS successfully moves the 4,4′-DDE peak away from the congested matrix region allowing for easier and more accurate identification and quantification.

ChromaTOF: Leading the Way in Advanced GCxGC Data Processing

LECO's pioneering efforts in GCxGC data processing have resulted in the most comprehensive software package available. Even the most demanding analytical samples will be easily characterized, resulting in increased component identification and laboratory productivity.

- User-defined classifications—peak grouping
- Bubble plots—peak intensity represented by circle radius
- Mass Spectral Scripts (visual basic programming) for enhanced spectral data-mining
- Statistical compare alignment tool
- Custom-generated reports
- Sample Comparison feature
- Built-in spreadsheets for advanced data-mining
- Data exporting for secondary software analysis
- Tools for 21 CFR Part 11 Compliance

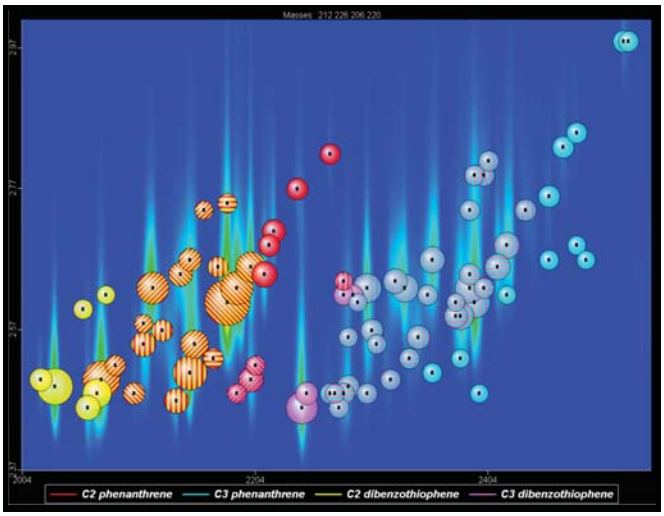

Figure 12. Bubble Plots are easily displayed to distinguish classifications as well as peak intensity.

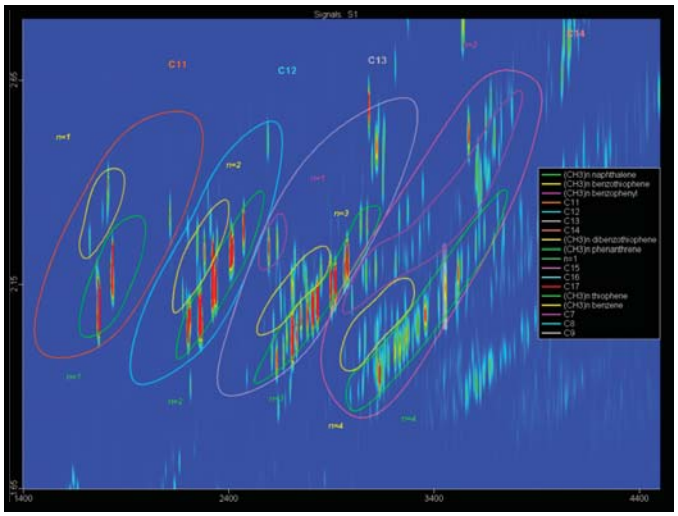

Figure 13. User-defined classifications identify regions containing sulfur and non-sulfur compounds found in this complex petroleum sample.

Training Classes

Get the most out of your LECO instrument with instrument-specific training classes offered from LECO. Typical classes feature a comprehensive overview of the theory of operation, method development, method optimization, and proper maintenance for each instrument class. A variety of advanced features are also presented, including calibration, user library creation, reporting, user fields, and optimization of both 1D and 2D chromatography. Classes also allow for networking opportunities and the ability to learn from other users of our GC-TOFMS, GCxGC, and GCxGC-TOFMS products. Attend classes at our facilities in St. Joseph, Michigan, or virtually anywhere with our online series of classes.

"Everyone is very knowledgeable (brilliant, if I may say!) and willing to help with any questions/problems. I am amazed at and extremely happy with the high level of service LECO provides."

~LECO Customer and Class Participant

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Delivering the Right Results

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