

## PEGASUS<sup>®</sup> HT High Throughput TOFMS

# LECO's PEGASUS<sup>®</sup> HT TOFMS

High Throughput Time-of-Flight Mass Spectrometer



## The solution to your analytical challenges

The Pegasus HT TOFMS combines LECO's Time-of-Flight Mass Spectrometer (TOFMS) with ChromaTOF<sup>®</sup> software to provide revolutionary Time-Compressed Chromatography, Complex Sample Resolution, Automated Peak Find, and True Signal Deconvolution<sup>®</sup> in a high throughput GCMS. No other system can match the Pegasus TOFMS for speed, accuracy, and proven reliability.

### ChromaTOF Workstation

- Windows<sup>®</sup>-based platform
- High-speed processor
- Large data storage capacity
- Remote diagnostics

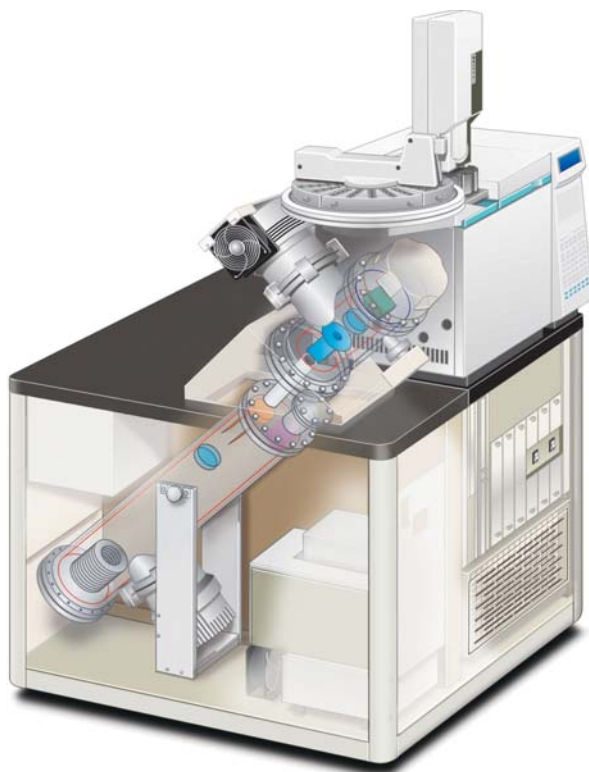
### Pegasus HT TOFMS

- Fastest spectral acquisition rate (500 Hz)
- Dynamic signal tracking
- Low-maintenance ion source
- Proven reliability

Patents include no. US4472631, US4490806, US5175430, US5367162, US5712480, IT1167562, WO9220435, WO8304326, WO9500236, EP540720, CA1225155. Other patents pending.



# The Power of LECO TOFMS



## Features

Continuous full-range mass acquisition rate up to 500 spectra/second (500 Hz)

Full-range mass sensitivity

Linear dynamic range of 4 orders of magnitude or more

Robust Never-Clean ion source

ChromaTOF software

Integrated control from ChromaTOF software

## Benefits

Ability to define the narrowest of GC and GCxGC peaks

Full-range mass spectral data for True Signal Deconvolution

Accurate identification of unknown and targeted compounds in complex samples

Ability to review archived data for new compounds outside the scope of the initial analysis

2 pg of Hexachlorobenzene on column produces signal-to-noise ratio  $\geq 10$  at mass 284

Accomplish in one run what other mass spectrometers require multiple runs to accomplish

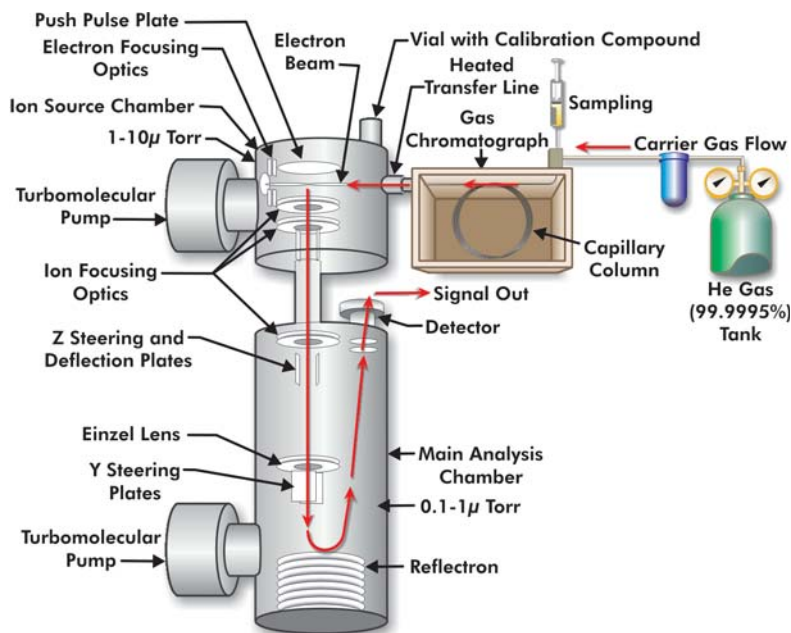
Analyze and quantitate real-life samples of varying concentrations in matrix

No laboratory down-time associated with source cleaning  
Proven reliability  
Higher productivity

Automated Peak Find and True Signal Deconvolution for fast/easy data analysis and clean library searches  
Custom report generation  
Environmental reporting packages available  
Comparison feature for fast/easy sample analysis and the ability to quickly determine quality lots

Agilent GC or LC instruments  
Multiple sample-handling accessories available, including LEAP, Gerstel, and Agilent  
Various available detectors (FID, ECD, SCD)  
Remote start, contact closures for other instrumentation  
Total system automation for maximum productivity

## Diagram of GC-TOFMS Instrument



## Fast Acquisition GCMS

Every laboratory knows time is money, and improved productivity is one way to generate greater profit. LECO combines its unrivaled Mass Spectrometer (500 Hz) detector with patented data-mining algorithms to produce the speed and resolution necessary to accomplish Time-Compressed Chromatography and Complex Sample Resolution. No other company in the world delivers both technologies to you in the same package.

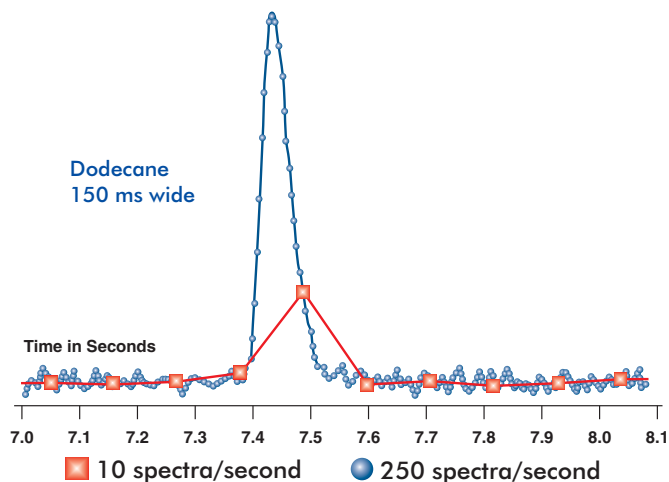
- Greater sample throughput by reducing run times
- Less sample degradation
- Faster method development
- No statistical under-sampling (associated with scanning detectors)
- Automated Peak Finding and True Signal Deconvolution

# World's Fastest Mass Spectrometer

## Up to 500 full-range mass spectra/second (500 Hz)

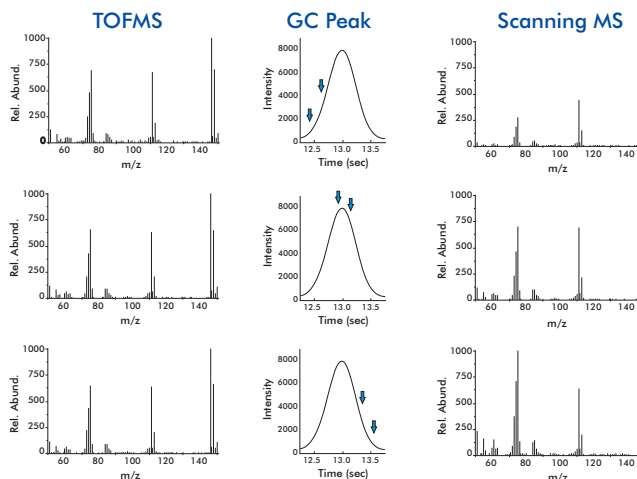
It is well agreed upon in the scientific community that a minimum of 10 data points across a fully-resolved chromatographic peak are needed for proper peak definition. However, 18-20 points are required for Automated Peak Find, True Signal Deconvolution, and proper peak identification and quantification in complex samples. The Pegasus TOFMS is capable of collecting 500 full-range mass spectra/second, making it the ideal detector for **Routine GC Analysis, High-Speed GC, Time Compressed Chromatography, and Comprehensive Two-Dimensional Chromatography (GCxGC)**. With user-defined collection rates up to 500 Hz, the Pegasus TOFMS can deliver sufficient data density to accurately characterize even the narrowest GC peaks.

### Acquisition Rate



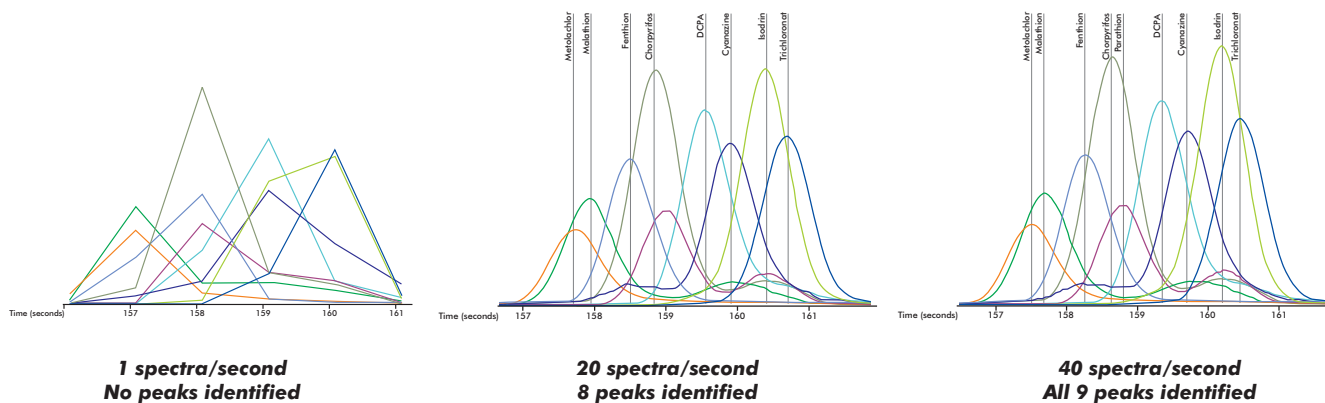
250 spectra/second was required to obtain the ideal 18-20 spectra across this Dodecane peak. 10 spectra/second, a common collection rate for other instruments, can distort peak shape, peak height, and apex location.

### Spectral Continuity



An inherent advantage of TOFMS with time-array detection is the complete absence of ion concentration biasing. With scanning instruments, the concentration in the chromatographic peak, and thus in the MS ion source, changes for each mass during a scan. If the concentration change is significant, spectral deconvolution of unknown peaks with significant chromatographic coelution is unreliable. TOFMS overcomes this limitation and provides a skewed-free spectra across the entire peak.

### Effect of Acquisition Speed on Automated Peak Find

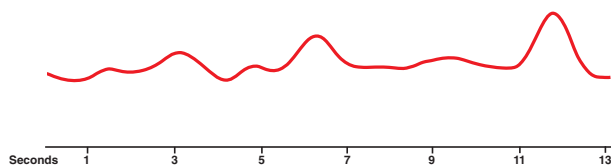


In this example, the ability to acquire data greater than 20 spectra/second (20 Hz) is necessary for automated peak identification and deconvolution of all 9 pesticides in the mixture.

Acquisition Speed without Spectral Continuity=Limited Deconvolution  
Spectral Continuity without Acquisition Speed=Limited Deconvolution  
Acquisition Speed and Spectral Continuity=True Signal Deconvolution!

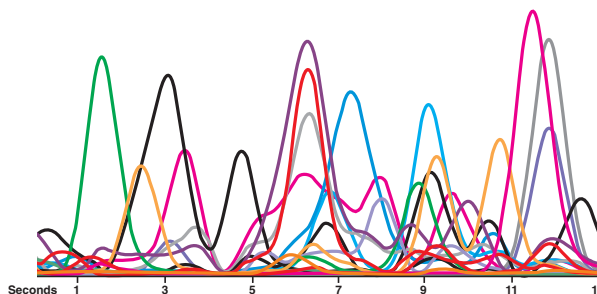
# Automated Peak Find and True Signal Deconvolution<sup>®</sup>

## Automated Peak Find



8 peaks are observed in this 13-second interval of the TIC.

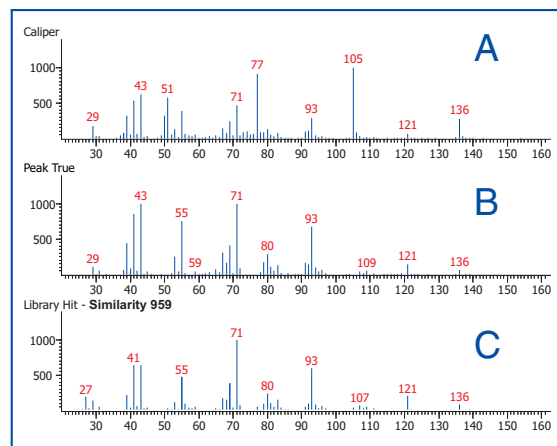
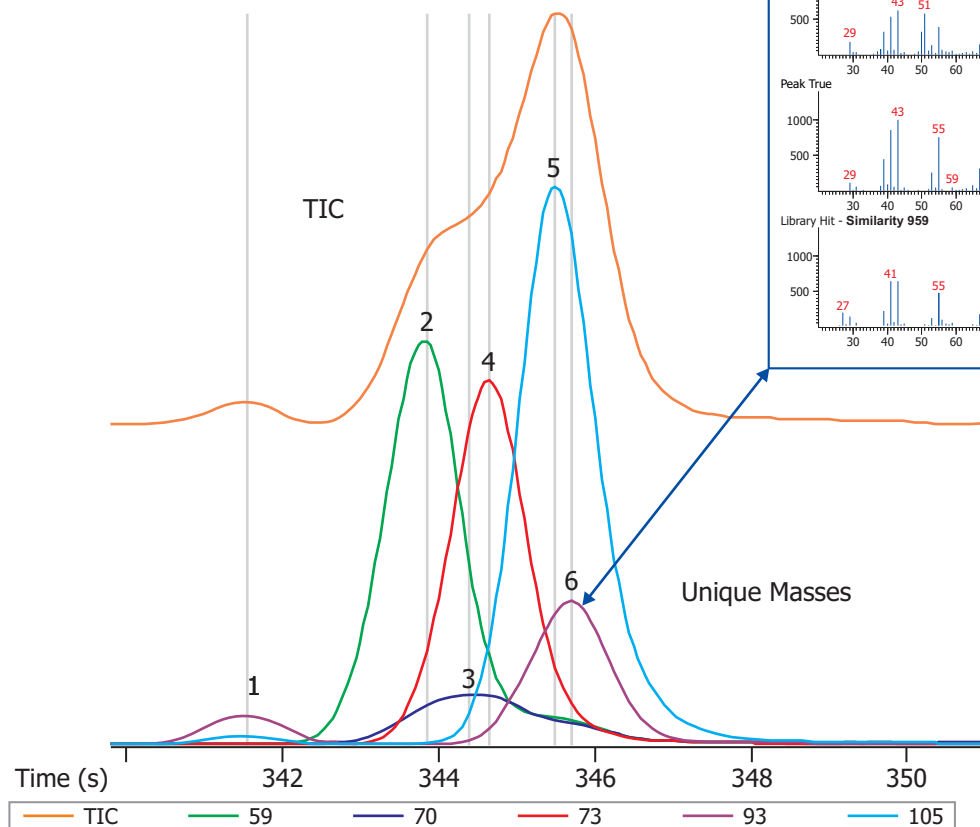
Detecting low-level unknown analytes is an extremely difficult task. Typically, the analyst is left to search the Total Ion Chromatogram (TIC), looking for small deviations in the baseline. The more complex the sample matrix the greater the background signal encountered in the TIC, causing the unknown analytes to be quickly lost in the background.



The Peak Find algorithm automatically detects 21 analytes in the same 13-second section of the chromatogram.

The Peak Find algorithm automatically locates all peaks in the chromatogram, when provided with only an expected chromatographic peak width and a signal-to-noise threshold. Coeluting analytes, peaks buried beneath the background of the TIC, and even small peaks buried beneath large matrix interferences are automatically detected and reported.

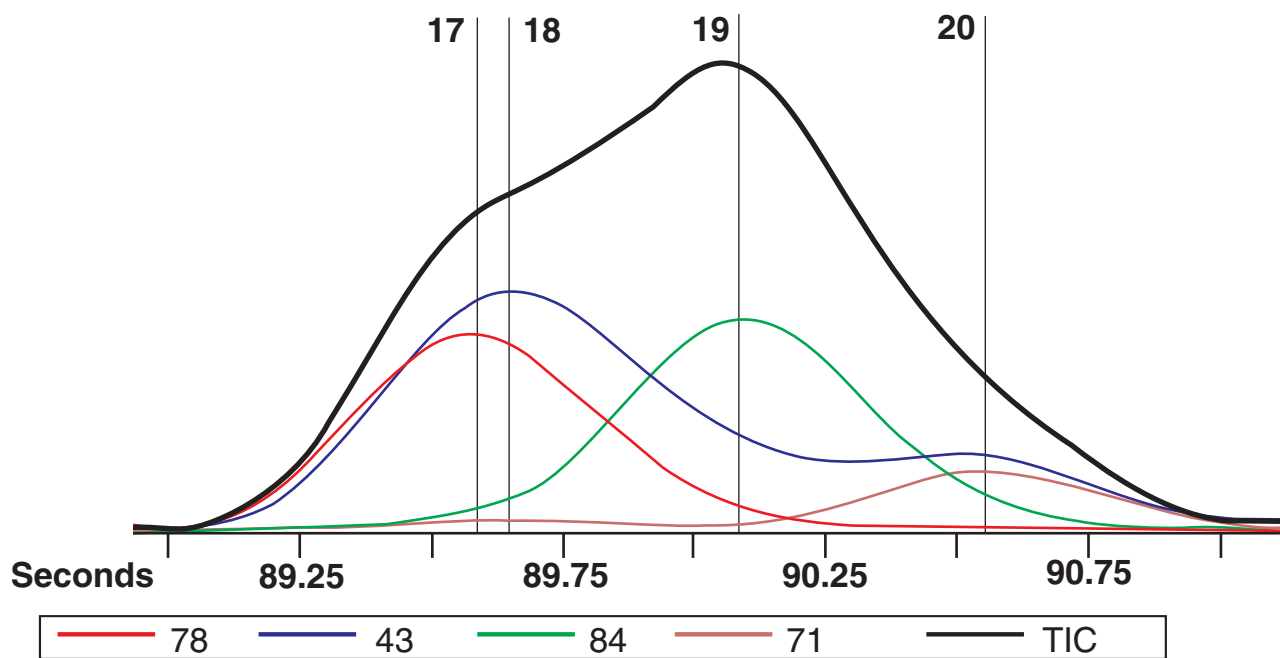
## True Signal Deconvolution (TSD)



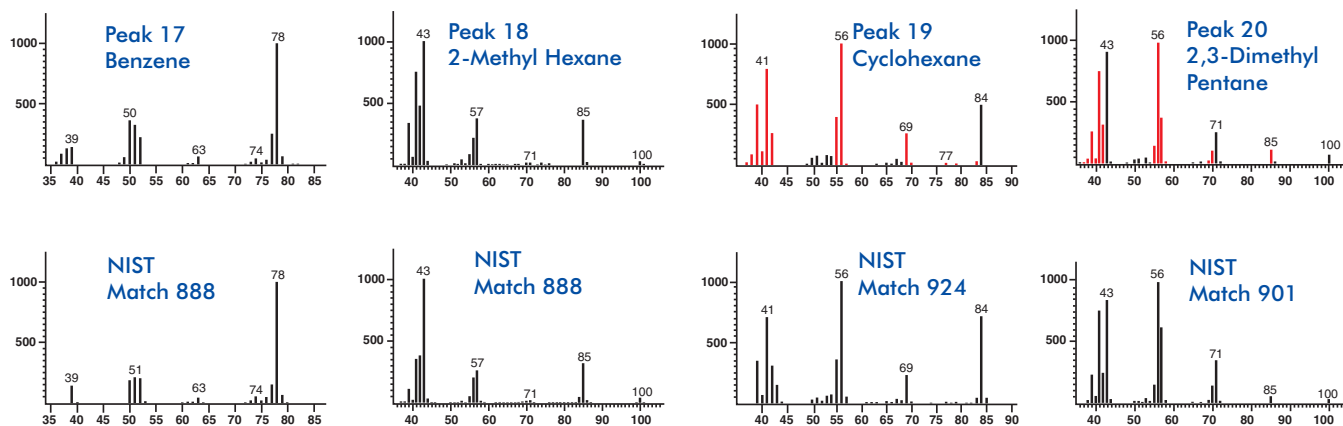
The TIC spectrum of Linalool (Peak 6) is automatically deconvoluted from five other coeluting peaks in this thermal desorption analysis of commercial liquid hand soap. The deconvoluted spectrum (B) is then matched against the NIST library (C) for improved spectral match and accurate compound identification. No other GCMS software delivers you the power of TSD and Automated Peak Find within a seamless software package.

## True Signal Deconvolution® (TSD®)

After the Peak Find algorithm has located all of the analytes, a mass spectrum for each analyte is automatically extracted free of interferences from the system background, matrix background, and coeluting analytes using True Signal Deconvolution. Even ions that are shared between coeluting analytes are accurately proportioned to provide you with a complete mass spectrum. The resulting spectrum is then used for analyte identification by spectral interpretation or by library search using any number of commercially available or operator-prepared databases.



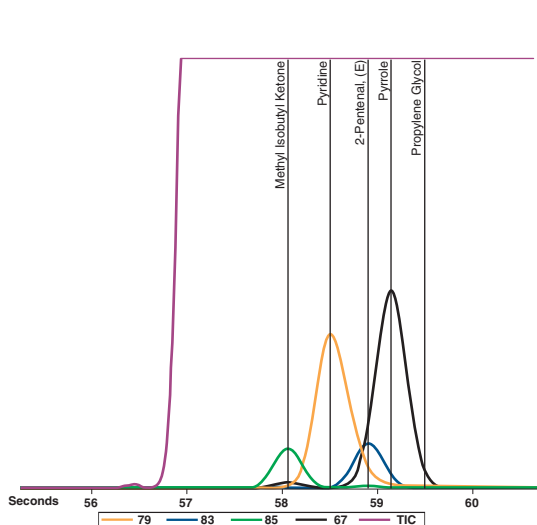
The Peak Find algorithm detects 4 analytes coeluting in this 2-second interval of the Naphtha Hydrocarbon TIC.



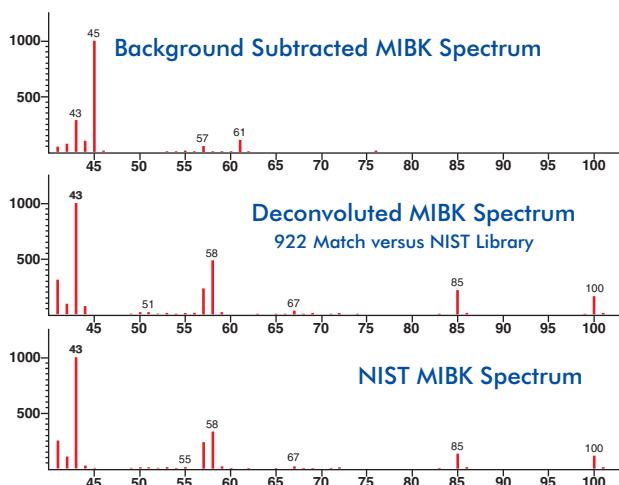
After True Signal Deconvolution, peaks 17 and 18 are detected and accurately identified by library search even though they are separated by only 0.07 seconds. Peaks 19 and 20 are accurately identified despite the high degree of shared signal (shown in red) observed in their mass spectra.

## Matrix Masking of Unknown Analytes

The Automated Peak Find and True Signal Deconvolution algorithms also work in detecting trace analytes in the presence of high matrix backgrounds. ChromaTOF software will uncover analytes never before observed by other GC-MS systems. The Pegasus has accurately detected and identified unknown trace analytes located beneath matrix interferences at concentration differentials of over 400,000 to 1. When complete sample characterization is a necessity, ChromaTOF software provides you with the answers.



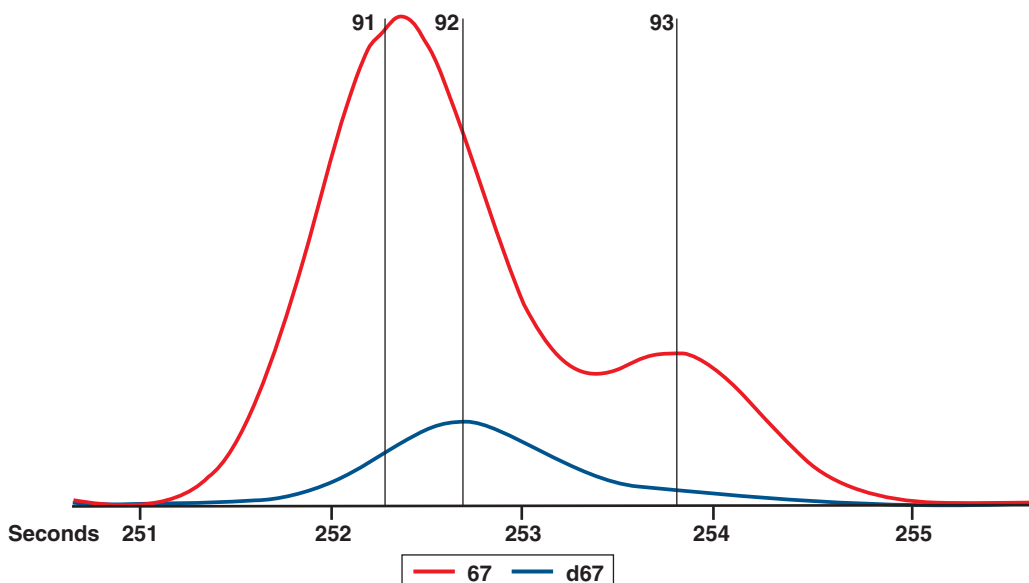
**Small, unknown analyte peaks are automatically detected beneath large matrix interferences.**



**The matrix masks the presence of MIBK when traditional background subtraction is used. The Peak Find and TSD algorithms accurately detect and identify the MIBK peak.**

## Deconvolution of Matrix-Masked Peaks

Matrix interferences may distort the peak shape of the selected quantification mass of a target analyte, impacting the accuracy of the peak area measurement. Creative baseline techniques such as the use of perpendicular drops, recalibrating on a new ion, modifying the chromatographic separation to resolve the interference, or modifying sample preparation procedures to remove the interference sacrifice accuracy and are very time consuming. ChromaTOF's True Signal Deconvolution algorithm accurately proportions shared ion signals between coeluting analytes. This same algorithm can also be used to remove matrix interferences by displaying only the ion signal contributed by the target analyte. Accuracy and precision are improved with no additional effort.

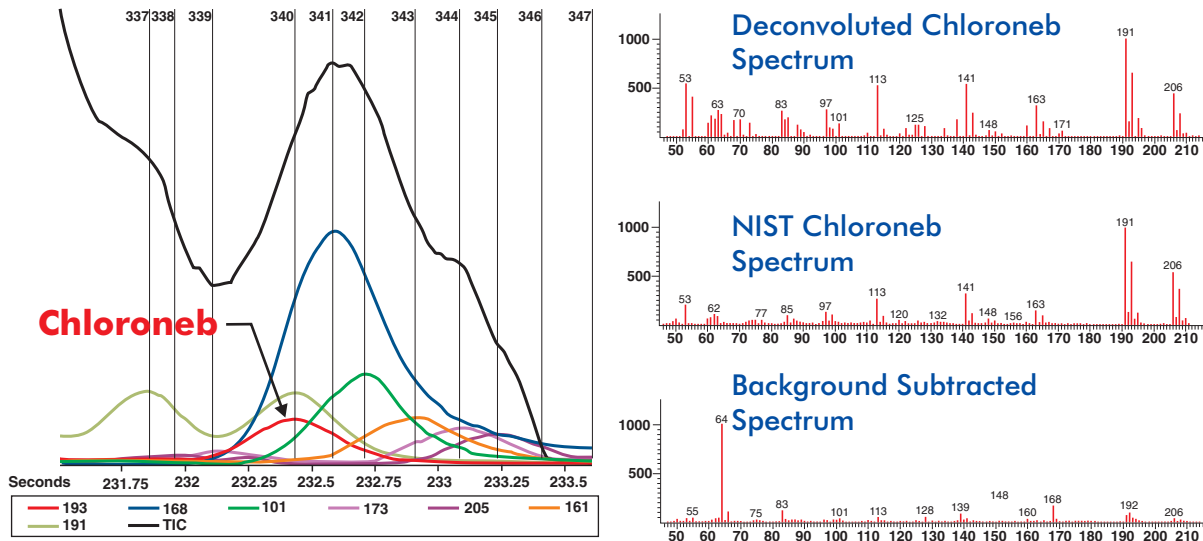


**The target analyte at peak marker 92 has been calibrated using m/z 67 (red). However, the matrix interferences at peak markers 91 and 93 also contain m/z 67 in their mass spectra. The TSD algorithm accurately proportions the shared signal to display only the m/z 67 contributed by the analyte at peak marker 92 (blue).**

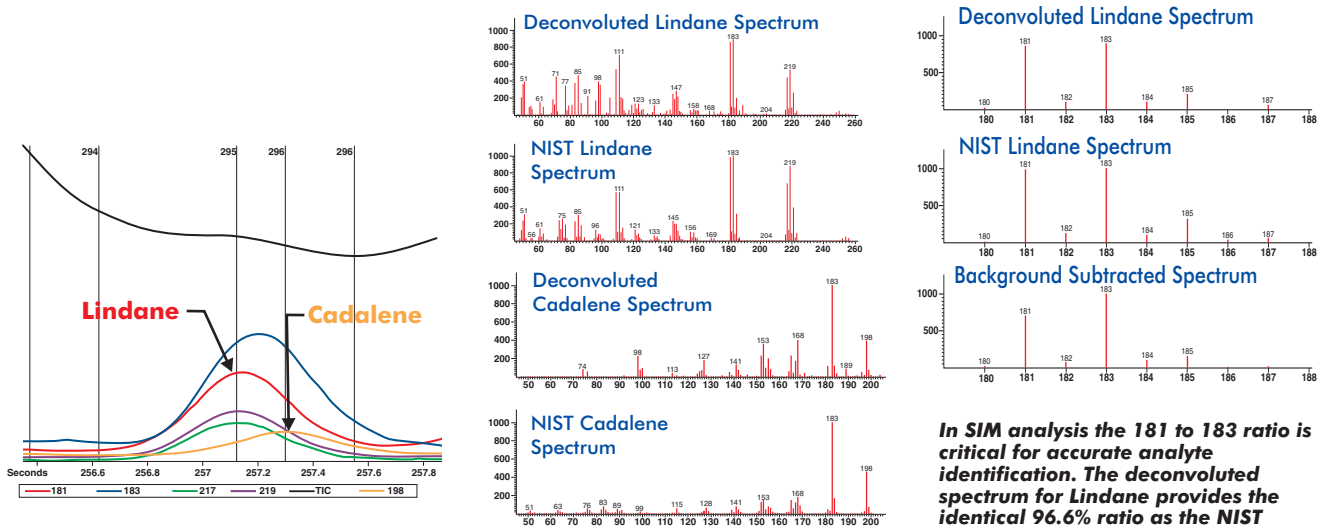
## Accurate Analyte Confirmation

Exact analyte confirmation is critical in quantitative analysis. LECO's Peak Find and True Signal Deconvolution algorithms accurately locate the target analytes and all coeluting interferences—providing you with extracted mass spectra free of matrix background. The risk of false-negative and false-positive reports is significantly reduced.

Selected Ion Monitoring (SIM) is used with other MS systems to manage matrix complexity. SIM, however, forfeits significant mass spectral information (important to accurate analyte confirmation) and has been shown to be less accurate than deconvolution. SIM provides enhanced sensitivity on target analytes only—while the Pegasus, with True Signal Deconvolution, provides you with enhanced sensitivity on all analytes in the sample.



**A possible Chloroneb peak (red) is detected beneath a significant concentration of matrix in the chromatogram shown on the left. The deconvoluted mass spectrum for Chloroneb (top) clearly matches the Chloroneb NIST spectrum (middle) for accurate analyte confirmation. Simple background subtraction provides much less information. Without deconvolution the Chloroneb would be reported as not present in the sample.**



**Lindane and Cadalene are detected as coeluting analytes beneath the background of the TIC.**

**Both Lindane (top) and Cadalene (bottom) are accurately identified by library search.**

**In SIM analysis the 181 to 183 ratio is critical for accurate analyte identification. The deconvoluted spectrum for Lindane provides the identical 96.6% ratio as the NIST library. The background subtracted spectrum (bottom) shows an erroneous 70.5% ratio due to the heavy contribution to the 183 ion by the coeluting Cadalene.**

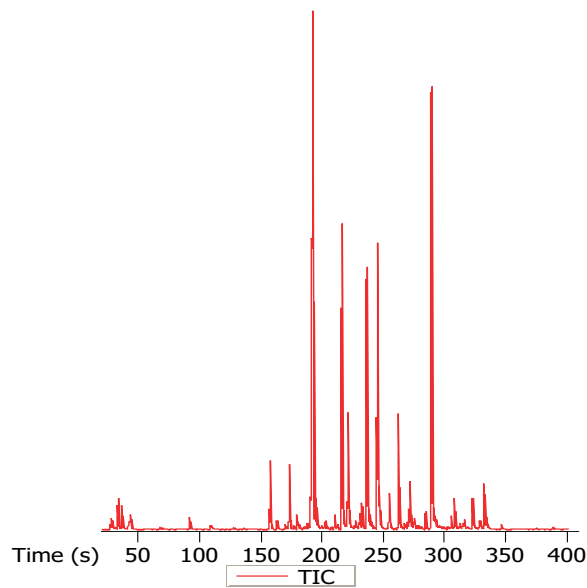


# Productivity Optimization

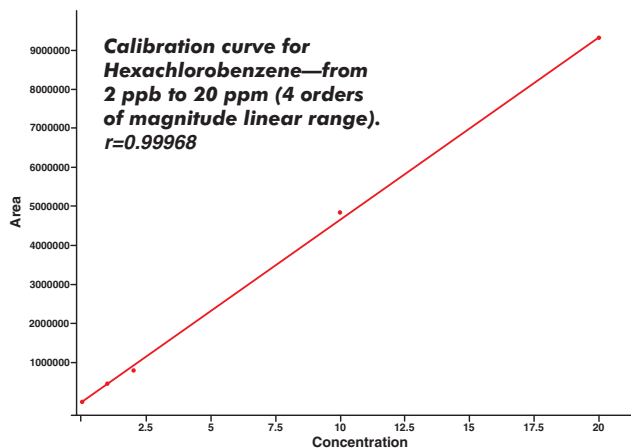
For enhanced laboratory productivity, all aspects of a designated method must work together to achieve optimal performance. The Pegasus HT TOFMS optimizes productivity and increases your laboratory throughput from start-to-finish by offering you a number of automated and easy-to-use accessories.

- Full sample preparation automation integrating LEAP and Gerstel component control into ChromaTOF
- High throughput GCMS utilizing optional Low Thermal Mass (LTM) column modules
- New optional industry-specific reporting packages for the environmental industry

LECO's patented Automated Peak Find and True Signal Deconvolution algorithms serve as a foundation for identifying a sample's true chemical content by automating the qualitative analysis process. These two algorithms are a standard part of our ChromaTOF software.



**Analysis of an essential oil in under 400 seconds. More than 100 compounds were identified.**

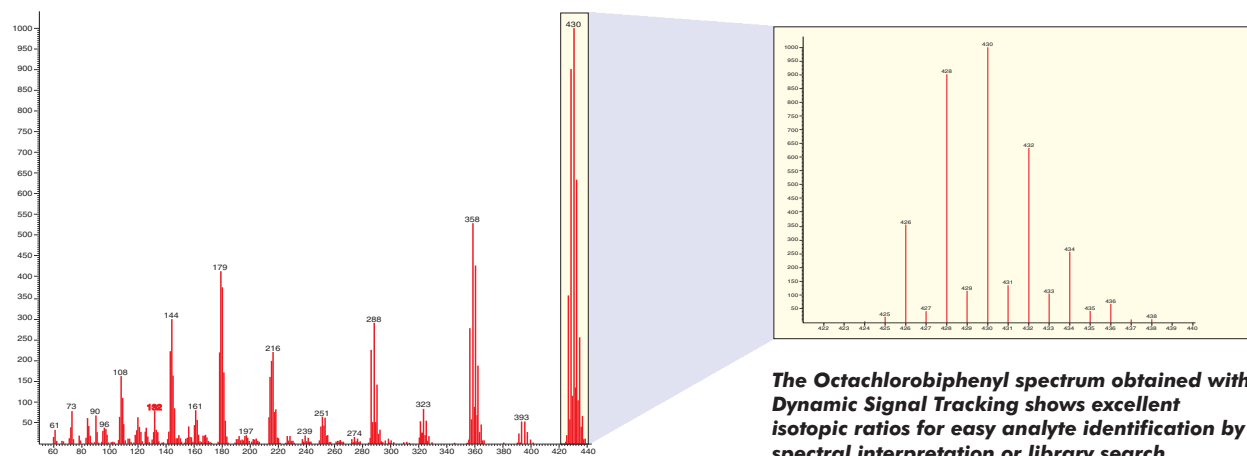


## Dynamic Range

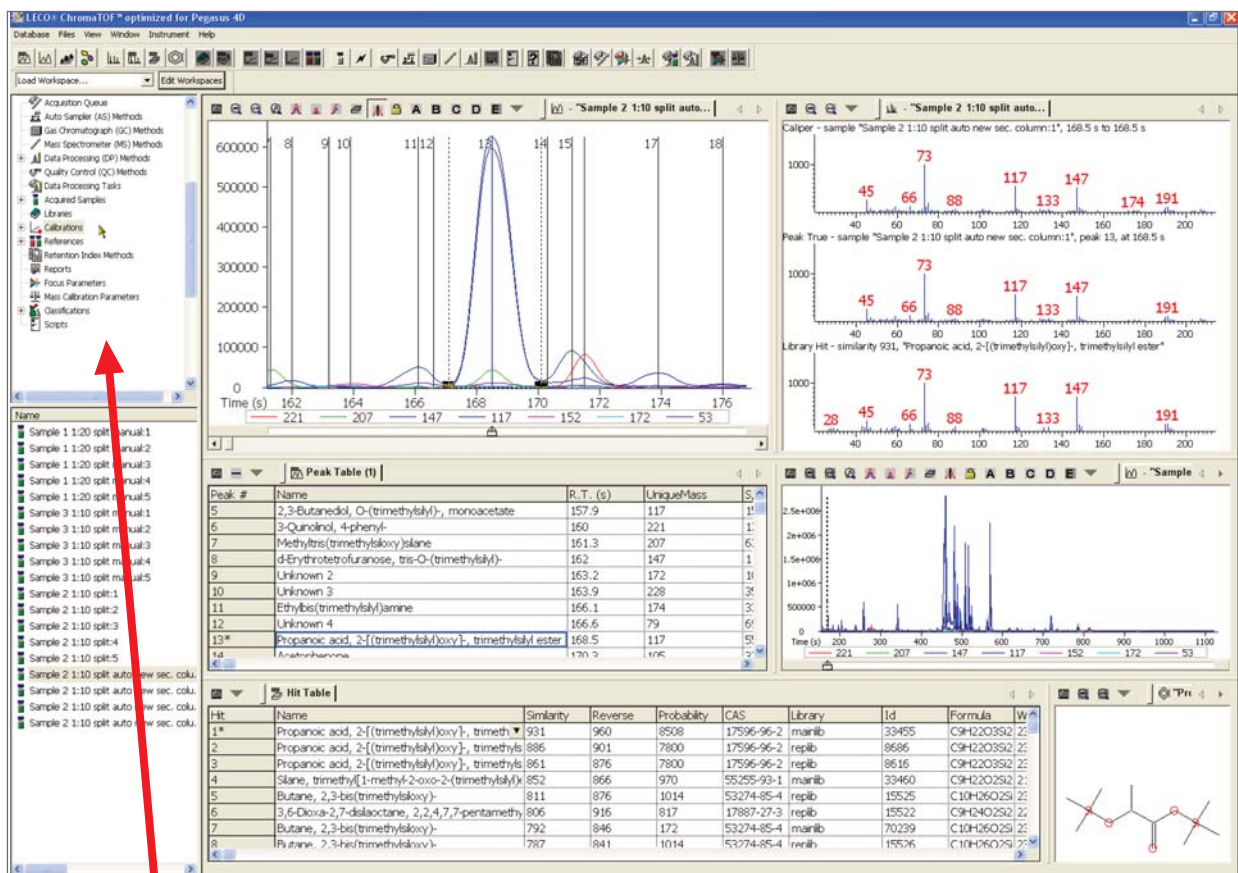
The Pegasus TOFMS offers you a linear dynamic range of 4 orders of magnitude or more. The range can be further lengthened using ChromaTOF's Extended Range Calibration algorithm. Decreasing the need for dilution and re-analysis of high concentration samples saves you analysis time. The Extended Range Calibration easily covers the capacity of any GC capillary column.

## Dynamic Signal Tracking

LECO's patented Dynamic Signal Tracking (DST) system ensures spectral quality and optimal mass resolution by correcting for minor deviations in ion flight time. Automatic Mass Defect adjustment ensures accurate isotopic spectral patterns, extends the dynamic range, and enhances system robustness.



# ChromaTOF® Software



## ChromaTOF Software

ChromaTOF software was designed with your laboratory in mind. With outstanding ease-of-use, ChromaTOF encapsulates the industry's most advanced qualitative and quantitative capabilities into one easy-to-use, seamless data-handling system.

- True Signal Deconvolution, Automated Peak Find, and Extended Range Calibration algorithms
- Semi-Quantitative Analysis for the reporting of non-calibrated compounds
- Automatic tuning within user-defined Quality Control methods
- Integrated control of a variety of sample handling options from Gerstel, LEAP, and Agilent
- Fully-integrated optional environmental report designer
- Customizable user interface
- Automatically export data to PDF, CSV, ANDI MS, NETCDF or Raw file formats

## System Reliability

To date, no Pegasus owners have ever needed to clean the ion source on their instruments. This unprecedented record is just one example of the incredible durability of the Pegasus HT TOFMS system. Should a problem ever arise, the ChromaTOF System Log automatically records all events in the mass spectrometer, simplifying the troubleshooting process. All events leading up to a performance issue can be reviewed by LECO's staff of trained Support Engineers. Multiple support resources can also be rapidly focused on any issue through the **SmartLine®** Remote Diagnostics service support program.

# LECO—Advanced Separation Science for the Working World

Every day around the world, LECO instruments continuously perform analyses for today's most complex applications. Whether you are analyzing samples in the food, flavor/fragrance, petroleum, environmental, or biotechnology (metabolomics) industries, we have an instrument configuration to meet your needs.



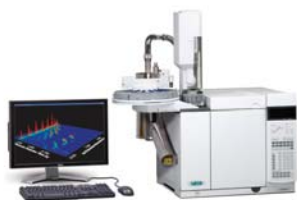
## Pegasus® 4D GCxGC-MS

- Pegasus, with 500 spectra/second, offers you the only MS detector capable of comprehensive two-dimensional GC (GCxGC)
- ChromaTOF software gives you the ability to take your sample characterization to the next level
- The ultimate in chromatographic resolution from the pioneer of GCxGC technology



## TruTOF® HT GCMS

- Continuous full-range mass acquisition rates up to 80 spectra/second (Fast GCMS)
- Electron ionization (EI) and chemical ionization (CI) source capabilities
- Environmental reporting software (standard)
- ChromaTOF software with Automated Peak Finding and True Signal Deconvolution for fast/easy data analysis and clean library searches



## GCxGC

- Offers you enhanced separating power for complex sample analysis
- Easy-to-use ChromaTOF software
- Classification software feature simplifies component identification
- Flame Ionization Detector (FID), Electron Capture Detector (ECD), and Sulfur Chemiluminescence Detector (SCD) available



## Unique® HT LCMS

- Accessible and affordable high-speed LC-TOFMS
- Compact benchtop TOFMS designed for complex sample analysis
- With collection rates up to 100 full-range mass spectra/second, the Unique is the best MS detector for the latest high-resolution/high-speed chromatographic applications
- Integrated control for high-speed Agilent 1200SL LC
- ChromaTOF Automated Peak Find and True Signal Deconvolution algorithms



Technical Research Center



Global Support Center



Life Science and Chemical Analysis Centre

## A Commitment to Quality and Service

LECO instruments are recognized for superior precision, speed, and ease-of-use. We are an international company with over 25 subsidiaries worldwide. Our global network of sales/support is dedicated to customer service and satisfaction, and our commitment to quality is further underscored with ISO-9001:2000 certification. We conform to CE quality and safety specifications, fully testing instruments at our on-site Compliance Testing Center.

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