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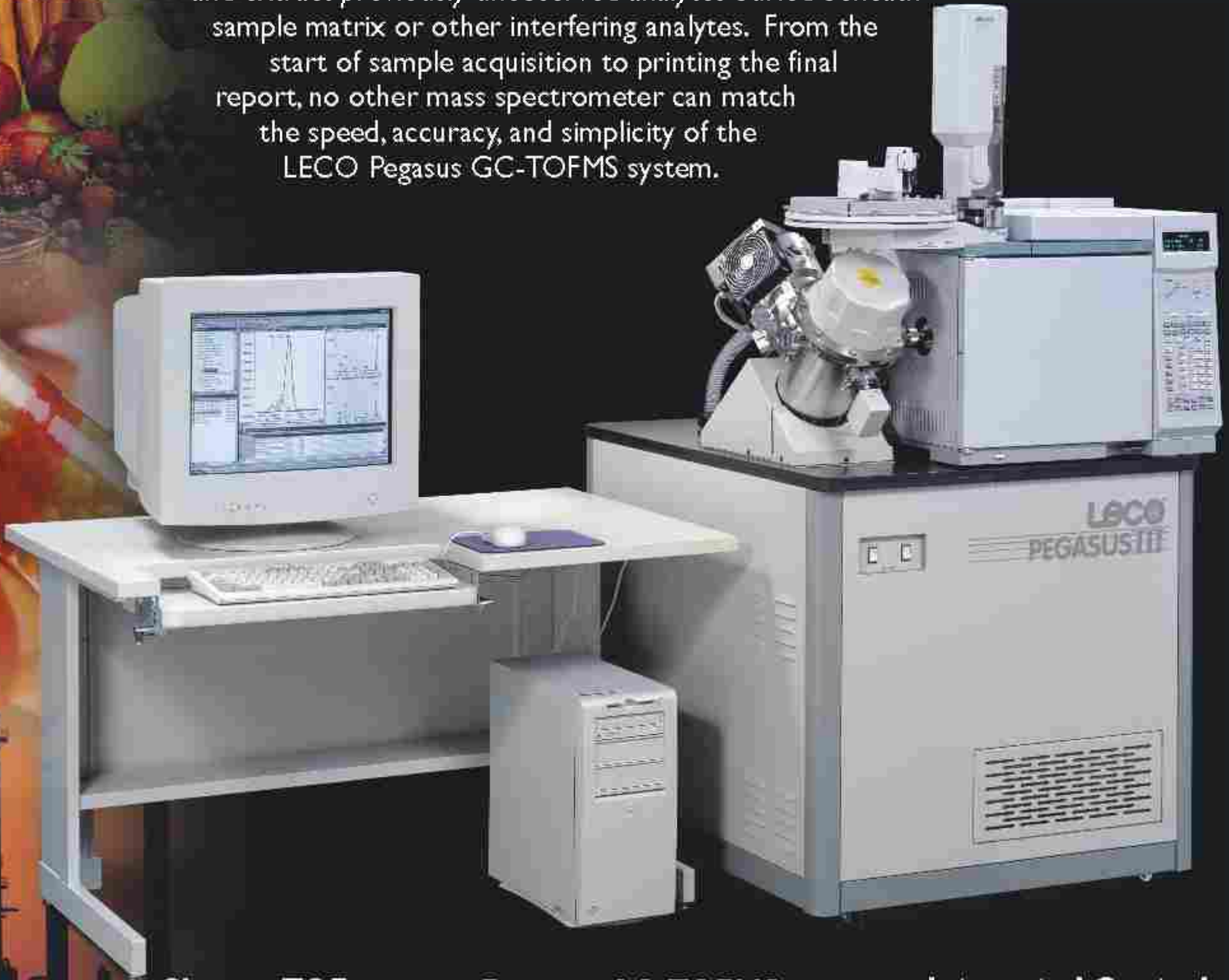
PEGASUS® GC-TOFMS

LECO *Pegasus*® GC-TOFMS... A Simple Solution for Complex Problems

The Pegasus GC-TOFMS provides simple and affordable solutions for reducing analysis times, locating target and unknown analytes masked by matrix interferences, and rapidly determining differences between complex samples. The Pegasus system combines proven LECO time-of-flight mass spectrometry technology with new ChromaTOF™ software to provide an unparalleled increase in laboratory productivity. Full range mass spectral acquisition rates of up to 500 spectra per second allow for significant reduction in chromatographic analysis time. Completely automated qualitative sample characterization, quantitative analysis, and/or intra-sample measurements can be completed in a fraction of the time required by manually-oriented processing systems. The ChromaTOF software package also offers sophisticated data-mining algorithms that automatically detect and extract previously unobserved analytes buried beneath sample matrix or other interfering analytes. From the start of sample acquisition to printing the final report, no other mass spectrometer can match the speed, accuracy, and simplicity of the LECO Pegasus GC-TOFMS system.



ChromaTOF Workstation

- Windows® Platform
- High speed processor
- Large data storage capacity
- Remote diagnostics

Pegasus GC-TOFMS

- Fastest reported spectral acquisition rate
- Dynamic signal tracking
- Low-maintenance ion source
- Proven reliability

Integrated Control

- Agilent® 6890 GC
- Agilent 7673 Autoinjector
- CTC CombiPAL™
  - Liquid Sampler
  - SPME
  - Headspace
- Gerstel® Inlet
- Remote start coordination

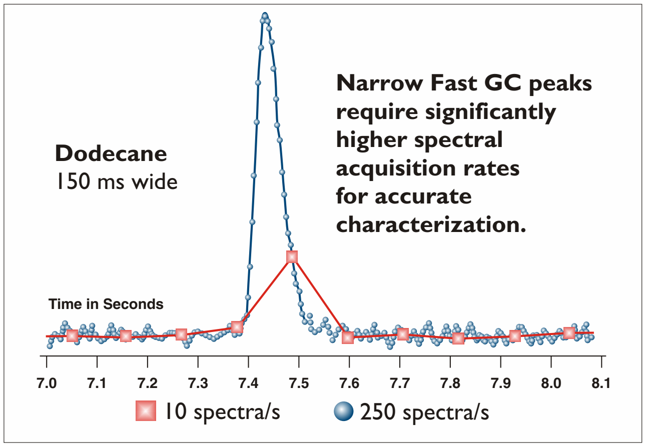
U.S. patents include no. 4,472,631 and no. 4,490,806. • Other patents pending.

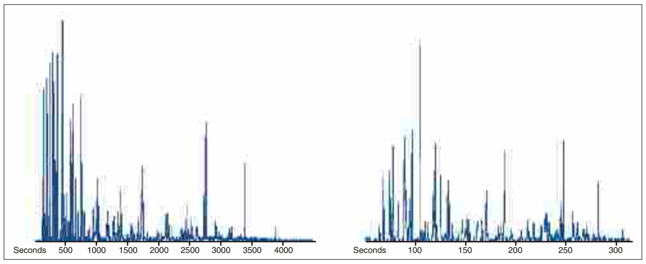
ChromaTOF Software

Pegasus' productivity enhancement does not stop at faster chromatographic analyses. Unique aspects of the ChromaTOF software package offer time savings in other parts of the analytical process as well. Fully automated Peak Find and Mass Spectral Deconvolution algorithms significantly reduce data processing time while providing considerably more comprehensive sample information. The ability to extract analyte information from beneath large matrix interferences offers the potential for additional time savings through the minimization of tedious sample preparation procedures. Finally, comprehensive quality control software provides complete automation of the entire analysis, guaranteeing that quality data will be collected while the instrument operates unattended.

Enhanced Productivity

Time is money and improved productivity generates greater profit for the laboratory. Reducing analysis time offers many productivity benefits including greater sample throughput, faster turn-around times for rush samples, faster method development, less problems with sample degradation, and fewer problems with statistical under sampling. The Pegasus GC-TOFMS is the world's fastest mass spectrometer reporting up to 500 full mass range spectra per second. Sufficient data density is obtained to accurately characterize even the narrowest GC peaks. The full power of Fast GC techniques may now be applied to GC-MS analyses—resulting in reductions of chromatographic analysis times of an order of magnitude or more.



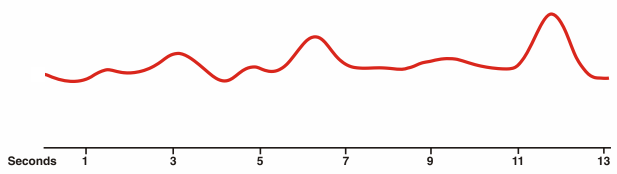


Traditional Naphtha Hydrocarbon analysis (left) yields 187 analytes in 75 minutes. The same analysis can be performed in 6 minutes using the Pegasus (right).

Completely Automated Qualitative Analysis

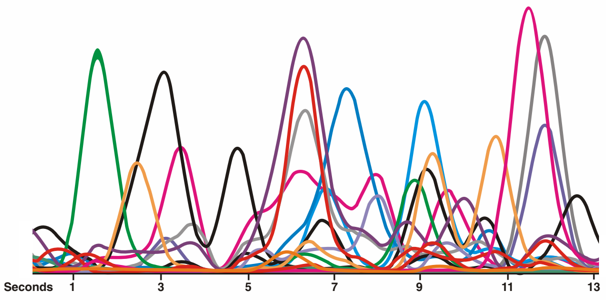
The unique Peak Find and Mass Spectral Deconvolution algorithms incorporated in the ChromaTOF software provide the means for completely automated qualitative analysis. These algorithms also serve as the foundation for other exclusive processing capabilities such as automated Sample Comparison algorithms, deconvoluted peak area measurements, and Isomer Quantification algorithms.

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 Current 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.

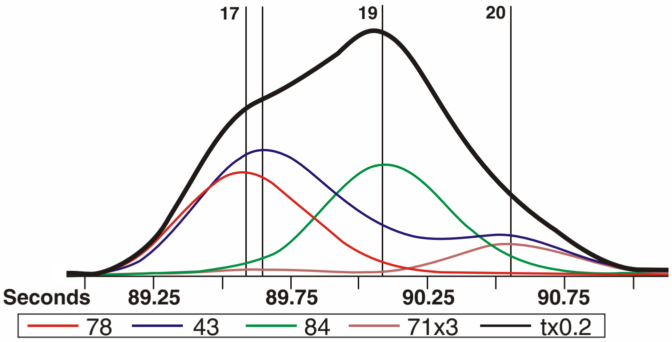


The Peak Find algorithm automatically detects 21 analytes in the same 13 second section of the chromatogram.

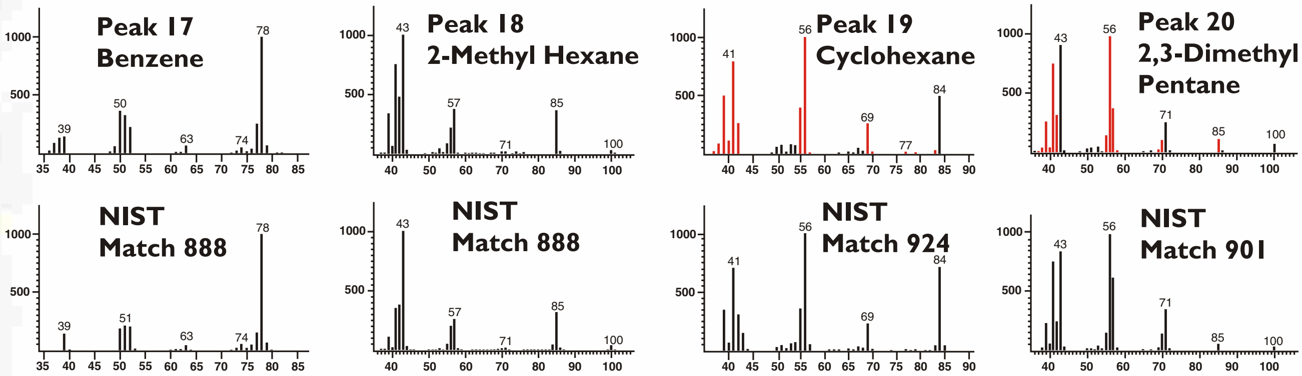
The Peak Find algorithm automatically locates all peaks in the chromatogram, even when provided with only an expected chromatographic peak width and a signal-to-noise threshhold. Coeluting analytes, peaks buried beneath the background of the TIC, and even small peaks buried beneath large matrix interferences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

Mass Spectral Deconvolution

After the Peak Find algorithm has located all of the analytes, mass spectra for each analyte are automatically extracted free of interferences from the system background, matrix background, and coeluting analytes. Even ions that are shared between coeluting analytes are accurately proportioned to provide 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.



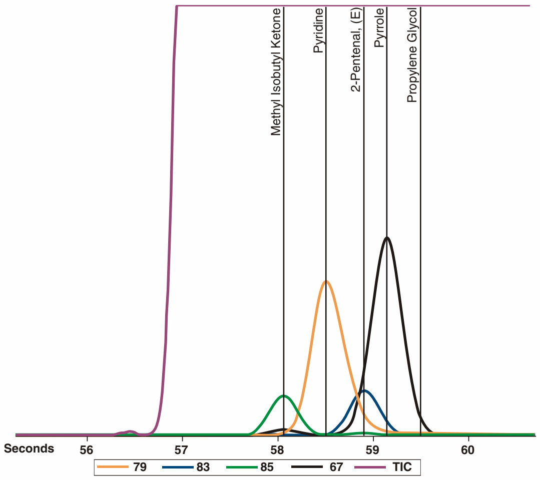
The Peak Find algorithm detects 4 analytes coeluting in this 2-second interval of the Naphtha Hydrocarbon TIC.



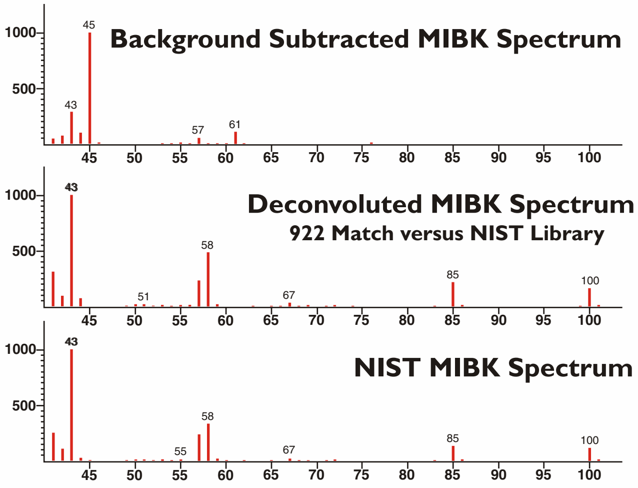
Peaks 17 and 18 are detected and accurately identified by library search even though they are separated by only 0.07 seconds. Peaks 19 and 20 are accurately identified despite the high degree of shared signal (shown in red) observed in their mass spectra.

Matrix Masking Of Unknown Analytes

The automated Peak Find and Spectral 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 the answers.



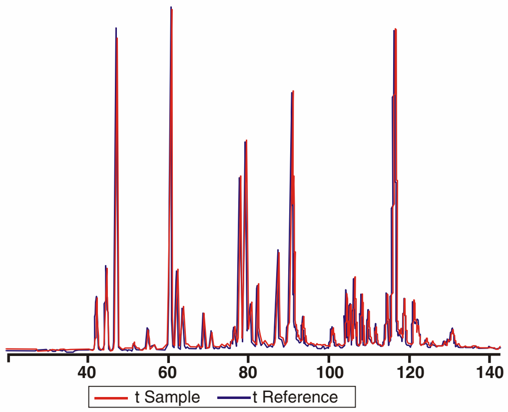
Small, unknown analyte peaks are automatically detected beneath large matrix interferences.



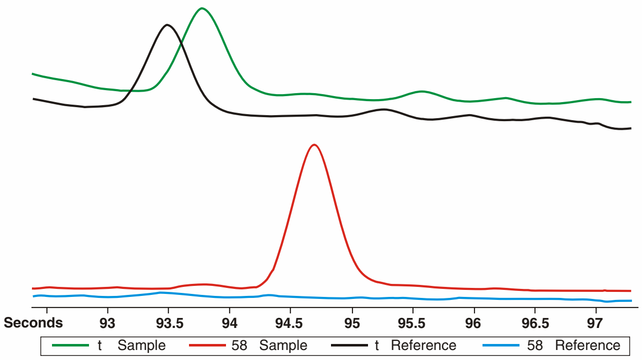
The matrix masks the presence of MIBK when traditional background subtraction is used. The Peak Find and Deconvolution algorithms accurately detect and identify the MIBK peak.

Automated Sample Comparisons

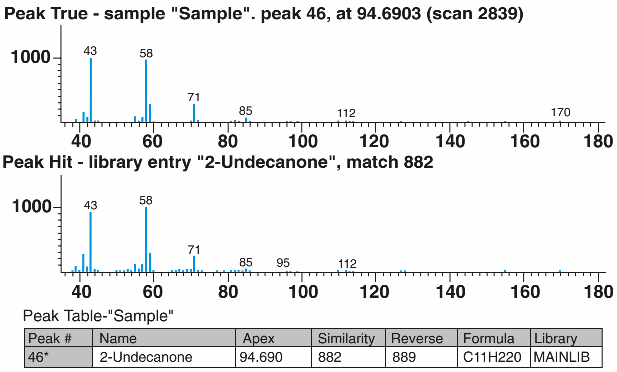
The ability to rapidly determine the differences between good and bad lots of material can save millions of dollars in production costs. LECO's automated Sample Comparison algorithm automatically compares a Sample to a Reference chromatogram to determine specific analyte similarities and differences. Three types of differences are detected, including omissions (analytes found only in the Reference), impurities (analytes found only in the Sample), and analytes found outside an analyst-defined concentration tolerance. The automated Peak Find and Spectral Deconvolution algorithms dig out the smallest differences from beneath the sample matrix—cutting the time to solve these difficult product quality problems by an order of magnitude or more.



No differences observed between the Sample and Reference TICs.



The automated Peak Find algorithm detects an analyte below the baseline of the TIC in the Sample that is not found in the Reference TICs.



Peak Table-"Sample"

Peak #	Name	Apex	Similarity	Reverse	Formula	Library
46*	2-Undecanone	94.690	882	889	C11H220	MAINLIB

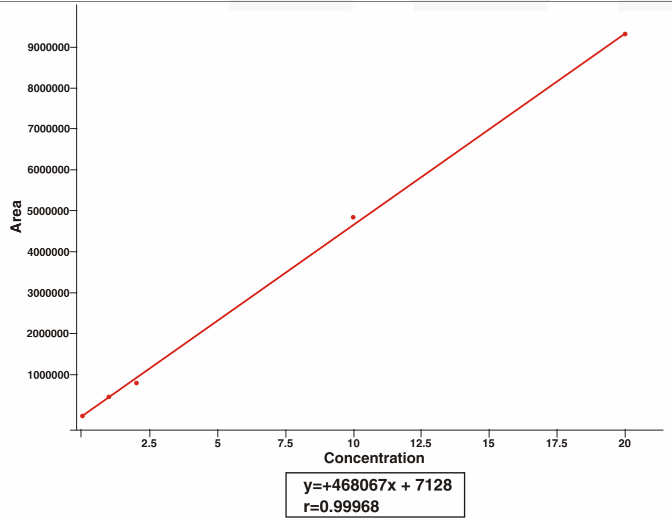
The deconvoluted spectrum for the Sample impurity is accurately identified by library search. The peak table is easily filtered to display all differences or any combination of impurities, omissions, or analytes detected outside the concentration tolerance.

Quantitative Analysis

The same features in the Pegasus that provide unique qualitative analytical capabilities can also be used to significantly enhance quantitative analyses as well. The Peak Find and Spectral Deconvolution algorithms slice through matrix interferences to provide significantly more accurate confirmation of target analytes. Once the analyte is correctly identified the broad dynamic range, the accurate deconvolution of chromatographic peak shapes, and the quantification of targeted isomers further enhance quantitative results.

Dynamic Range

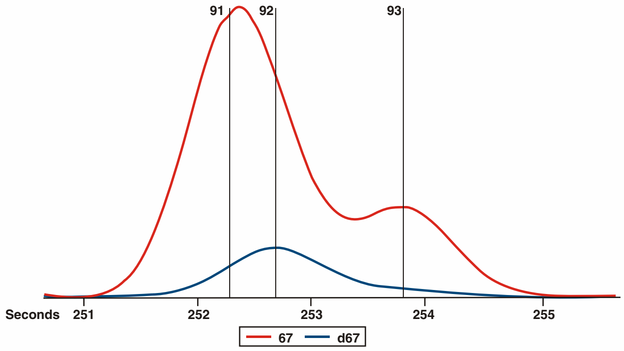
The Pegasus offers a linear dynamic range of 4 orders of magnitude or more. The range can be further extended using ChromaTOF's unique Dual Calibration Range algorithm. Decreasing the frequency of dilution and reanalysis of high-concentration samples saves analysis time and the extended calibration range easily covers the capacity range of any GC capillary column.



Calibration curve for Hexachlorobenzene—from 2 ppb to 20 ppm (4 order of magnitude linear range).

Deconvolution of Chromatographic Peak Shapes

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. The ChromaTOF Spectral 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.

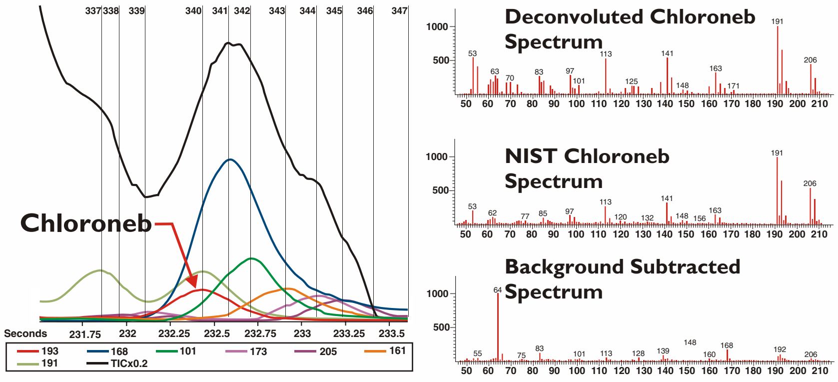


The target analyte at peak marker 92 has been calibrated using m/z 67 (red). However, the matrix interferences at peak markers 91 and 93 also contain m/z 67 in their mass spectra. The Spectral Deconvolution algorithm accurately proportions the shared signal to display only the m/z 67 contributed by the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

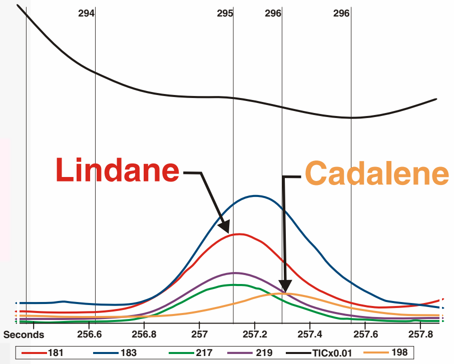
Accurate Analyte Confirmation

Exact analyte confirmation is critical in quantitative analysis. The Peak Find and Spectral Deconvolution algorithms accurately locate the target analytes and all coeluting interferences—providing extracted mass spectra, free of matrix background. The risk of false negative and false positive reports is significantly reduced.

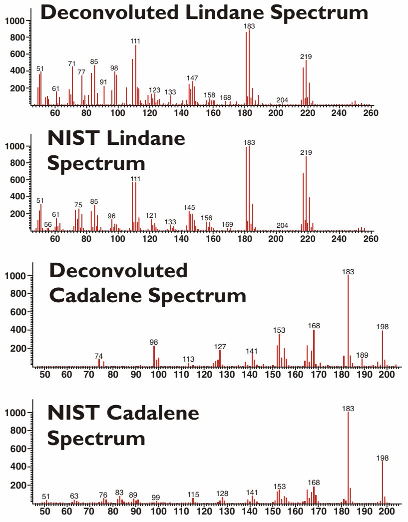
Selected Ion Monitoring (SIM) techniques or MS-MS may be used with other MS systems to manage matrix complexity. SIM forfeits significant mass spectral information (important to accurate analyte confirmation) and has been shown to be less accurate than deconvolution. Both MS-MS and SIM provide information on target analytes only—while the deconvolution approach provides information about all analytes in the sample.



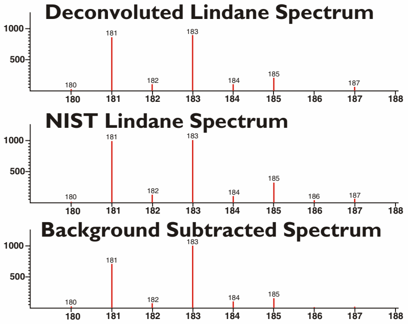
A possible chloroneb peak (red) is detected beneath a significant concentration of matrix in the chromatogram shown on the right. The deconvoluted mass spectrum for chloroneb (top) clearly matches the chloroneb NIST spectrum (middle) for accurate analyte confirmation. Background subtraction at the apex of the chloroneb peak provides the bottom spectrum. 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.



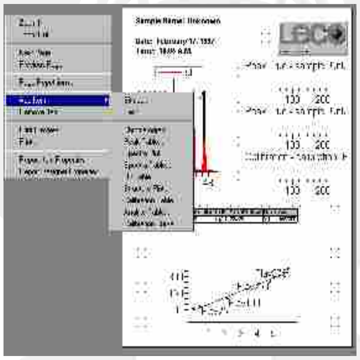
In SIM analysis the 181 to 183 ratio is critical for accurate analyte identification. The deconvoluted spectrum for Lindane provides the identical 96.6% ratio as the NIST library. The background subtracted spectrum (bottom) shows an erroneous 70.5% ratio due to the heavy contribution to the 183 ion by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

Total System Automation

Complete automation from sample injection through the generation of the sample report further maximizes laboratory productivity. The ChromaTOF software provides integrated control for the Agilent 6890 GC and 7673 Autosampler, as well as the CTC CombiPAL liquid injection, Solid Phase Micro Extraction (SPME), and Static Headspace modules. Automated data processing methods are easily added to the acquisition sequence for immediate processing following the completion of the data collection. Easy-to-use custom report design software allows for the preparation of a near infinite number of report formats. A variety of automated data export features ensures that the sample information is quickly routed to the appropriate destinations.

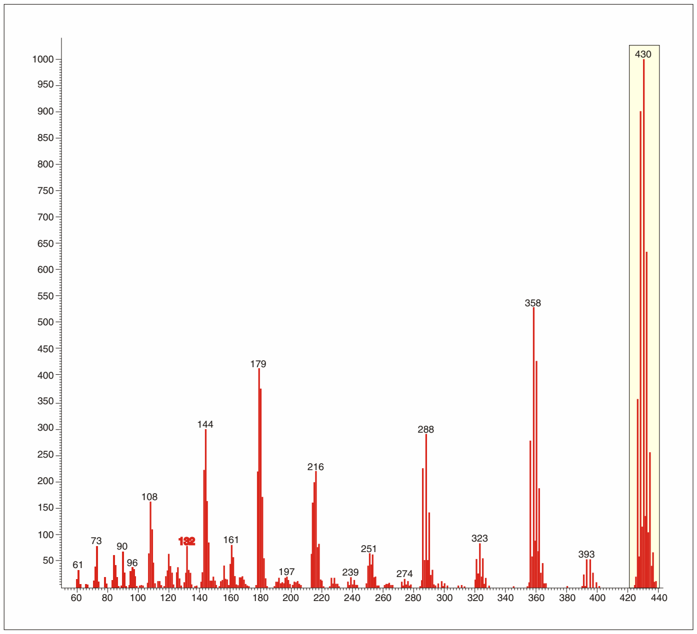
To ensure optimum productivity and data quality, a Quality Assurance package is provided in the ChromaTOF software. Instrument Optimization, Blank, Calibration, Peak Tailing, MS Tune Checks, Retention Index, and Internal Standard tests—as well as system optimization routines can all be evaluated at user-defined intervals to insure data quality.

Automated data processing methods are easily established by simply selecting the desired processing options.



Custom reports are created by a simple click, drag, and drop mechanism.

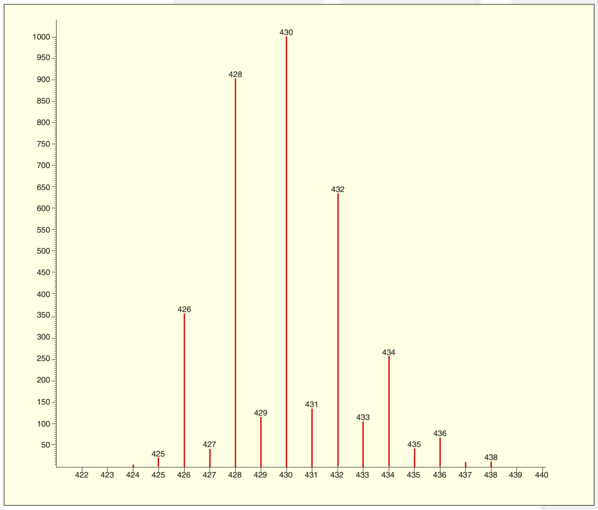
Simple fill-in menus allow for effortless configuration of Quality Assurance criteria.



The Octachloro PCB spectrum obtained with Dynamic Signal Tracking shows excellent isotopic ratios for easy analyte identification by spectral interpretation or library search. See detail at right.

Dynamic Signal Tracking

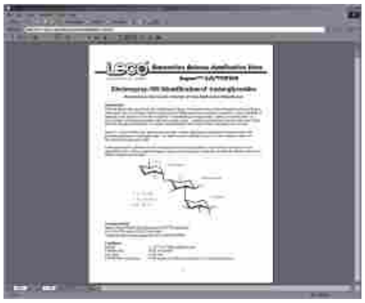
LECO's patented Dynamic Signal Tracking (DST) system ensures spectral quality by correcting for minor deviations in ion flight time to insure optimal mass resolution. Automatic mass defect adjustment to ensure accurate isotopic spectral patterns, an extended dynamic range, and enhanced system robustness are just a few of the advantages provided by DST.



System Reliability

To date, no Pegasus owners have ever needed to clean the ion source. This unprecedented record is just one example of the incredible durability of the Pegasus GC-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 problem are recorded for review by LECO's staff of trained Support Engineers. Multiple support resources can also be rapidly focused on any problem through the remote diagnostics system provided with every Pegasus system.

LECO's Mobile Demonstration Laboratory tours throughout North America year-round, bringing the Jaguar and Pegasus TOFMS instrumentation directly to your location. A ten-seat auditorium provides a comfortable atmosphere to discuss all aspects of the instrumentation. Skilled personnel are available to demonstrate these products and provide consultation regarding applications. The relaxed and private setting provides an excellent opportunity for a thorough introduction to LECO Time-of-Flight technology. Please contact your local LECO Separation Science Sales Engineer to arrange a demonstration at your facility.



www.leco.com

LECO's website offers a wealth of information on software updates, new products and consumables, catalogs, customer newsletters, technical articles, and much more. A complete library of TOF application notes is accessible with a click of the mouse! The site's straightforward design make it easy for you to find the information you need quickly.

Jaguar LC-TOFMS

The unique combination of speed and performance make LECO's new benchtop TOFMS one of the most versatile MS systems available for liquid sample analysis. Rapid acquisition rates of 100 spectra/second provide the data density required to support any of the latest fast separation techniques. Unmatched detection limits of 500 attamoles/spectrum or better, along with accurate mass measurement (within 5 ppm) greatly simplifies even the most demanding applications. Backed by a dedicated team of service application specialists, this affordable, compact LC-MS system is the perfect fit for any laboratory.

LECO subsidiaries span the globe so we can be there when you need us.

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