



UNIQUE[®] HT High Throughput TOFMS

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Affordable High-Speed LC-MS Technology from LECO



The new Unique HT TOFMS is the most sensible solution for your high-speed and complex sample analysis needs. The high-speed MS detector provides the data density required to support current and future advances in high-speed liquid chromatography. The Unique HT TOFMS bridges the gap between entry-level scanning MS technology and expensive hybrid technology. Capabilities include comprehensive spectral coverage for unbiased detection of both known and unknown analytes and >3 orders of magnitude linear detector response for high sensitivity detection. Industry-leading ChromaTOF[®] software provides fully integrated control of the Agilent 1200SL LC hardware and automated data processing tools to quickly transform data into results. These features have been integrated into an extremely cost-effective instrument, ideal for your food/food, metabolomics, and environmental applications.

Accurate Analyte Assignment

Whether confirming the presence of targeted compounds or analyzing unknowns in complex samples, the Unique HT TOFMS provides the tools necessary to achieve the results you expect. The TOFMS detector provides comprehensive spectral coverage for unbiased detection of known and unknown analytes within a sample. Peak Find and True Signal Deconvolution[®] algorithms automate the tedious task of confirming the presence of peaks. Accurate mass measurements to within 15 ppm combined with automated isotope pattern comparison, adduct/fragment ion deconvolution, and other filtering tools provide adequate data for formula calculation or automated library searching. Results are delivered in an easy-to-use, fully customizable, and context-sensitive user interface.

Excellent Sensitivity

The Unique HT TOFMS provides you with the sensitivity and wide dynamic range required for analysis of complex samples. A linear dynamic range of >3 orders of magnitude provides you with the ability to detect low ppb and high ppm analytes within the same sample. Routine electrospray operation for high-flow LC applications yields a Reserpine detection limit of 10 pg on-column or better. Improved sensitivity minimizes the need for tedious sample pre-concentration procedures prior to analysis. Sensitivity also allows smaller quantities of sample to be used, a tremendous benefit in sample-limited applications.

- Accessible, affordable high-speed LC-TOFMS
- Compact benchtop TOFMS designed for complex sample analysis
- High-speed, high dynamic range multi-channel data system
- ChromaTOF Automated Peak Find and True Signal Deconvolution algorithms
- Fully-integrated control for the high-speed Agilent 1200SL LC



High Throughput LC-TOFMS

Ultra-Fast Mass Spectrometry

It is well agreed upon in the scientific community that a minimum of 10 data points across a fully-resolved chromatographic peak is needed for proper peak definition. However, 18-20 points are required for proper deconvolution, peak identification, and quantification in complex samples. Given that the Unique HT TOFMS detector is the only MS detector capable of collecting more than 20 full-range mass spectra/second; it is the ideal detector for routine LCMS Analysis, High Throughput LCMS, and Complex Sample Characterization. Additionally, with user-defined collection rates up to 100 Hz, the Unique HT TOFMS is the only MS detector capable of properly defining the peaks generated by the latest high-speed liquid chromatography technology.

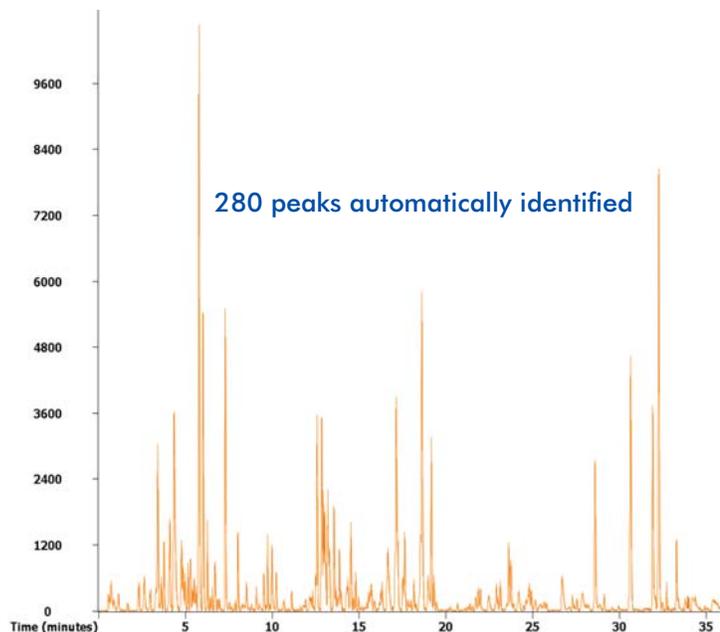


Figure 1 shows a complex Metabolomics sample separated using ultra high pressure LC. More than 280 peaks were automatically found and deconvoluted. Data was produced and provided courtesy of David Huhman and Lloyd Sumner, The Samuel Roberts Noble Foundation.

Effect of Acquisition Speed on Automated Peak Find

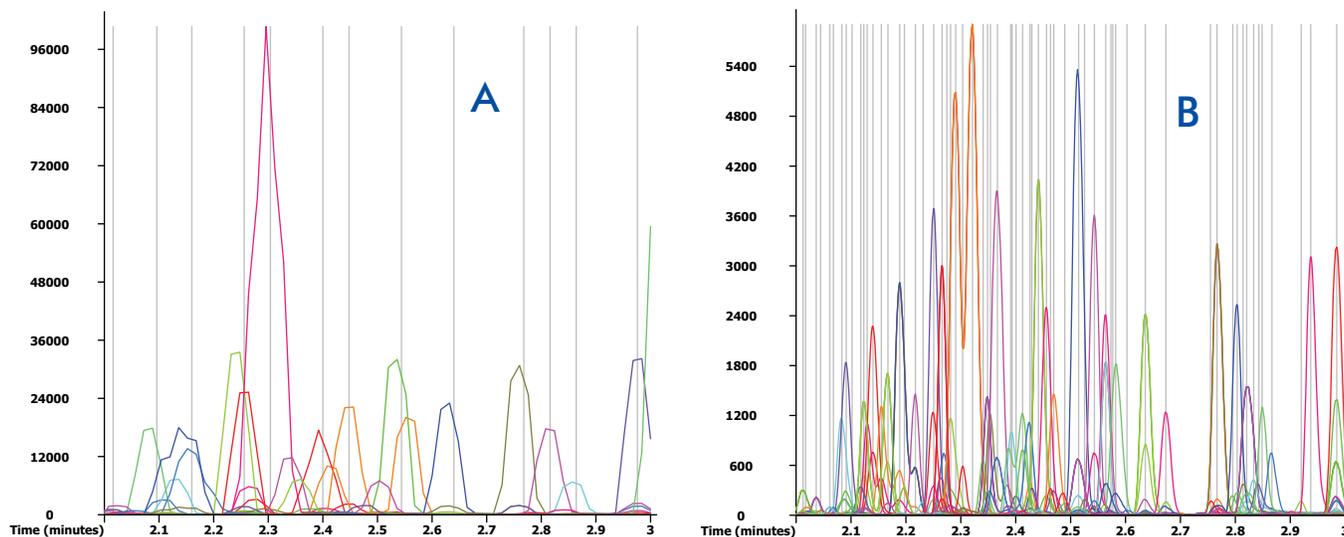


Figure 2 shows the effect of proper acquisition speed on peak shape and LECO's Automated Peak Find algorithm. Chromatogram A was collected at 1 spectra/second resulting in poor peak shape and only 13 peaks automatically found and identified. Chromatogram B, however, was collected at 25 spectra/second and resulted in superior peak shape which assisted in the detection of greater than 60 peaks for the same data.

Spectral Deconvolution

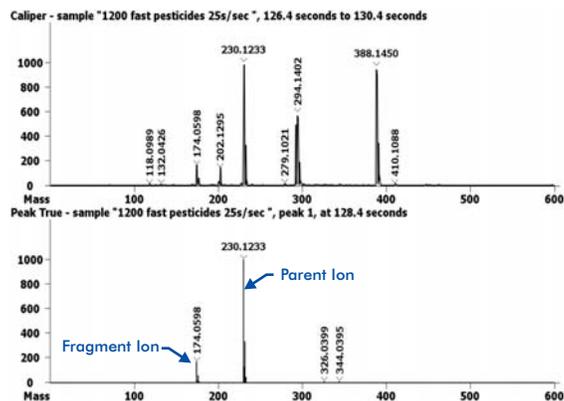
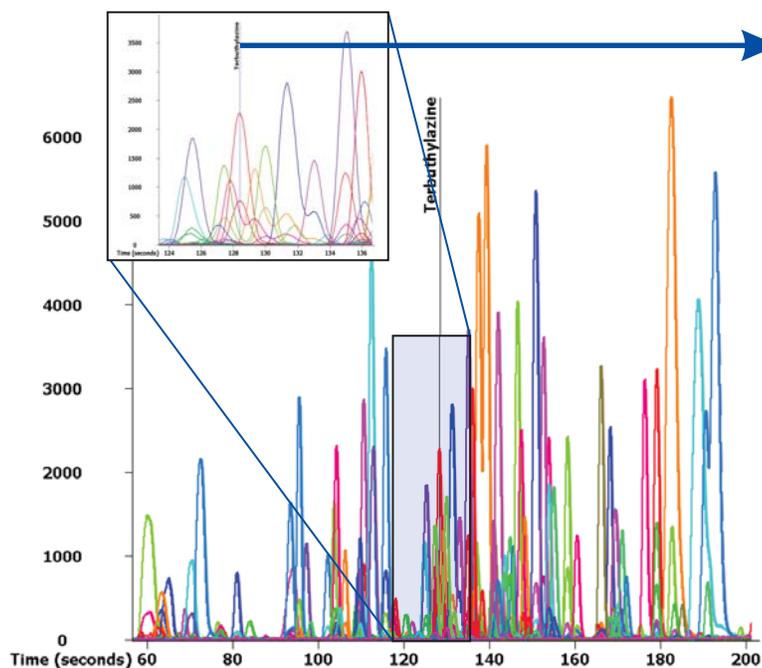
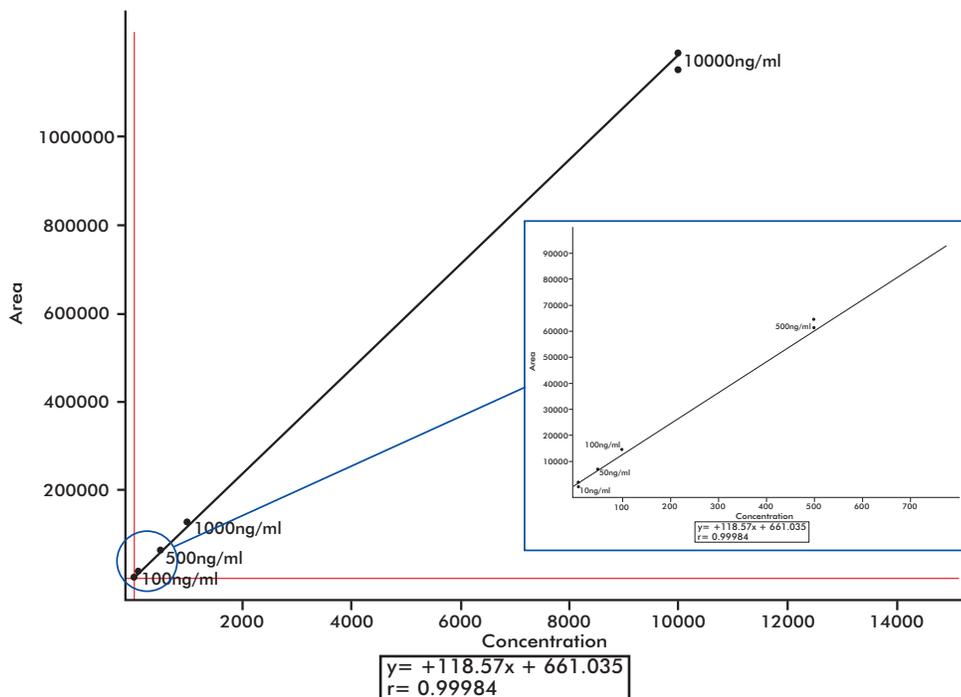


Figure 4. Mass Spectrum for Terbutylazine, before and after deconvolution.

Figure 3 (at left) shows Automated Peak Find results for a complex pesticide mixture. Once found, target compounds can be identified and extracted from the complex sample. The mass spectrum for Terbutylazine is shown above in Figure 4. Note that the deconvoluted Peak True spectrum is free of interfering masses and only shows parent and fragment ions of the selected compound.

Upon Automated Peak Finding, the True Signal Deconvolution algorithm automatically extracts accurate mass spectra—free of interferences from matrix background or coeluting analytes—for every cited peak. Automatic association of fragment ions, adduct ions, and molecular ions of varying charge-states to a single mass spectrum greatly simplifies the analyte confirmation process.

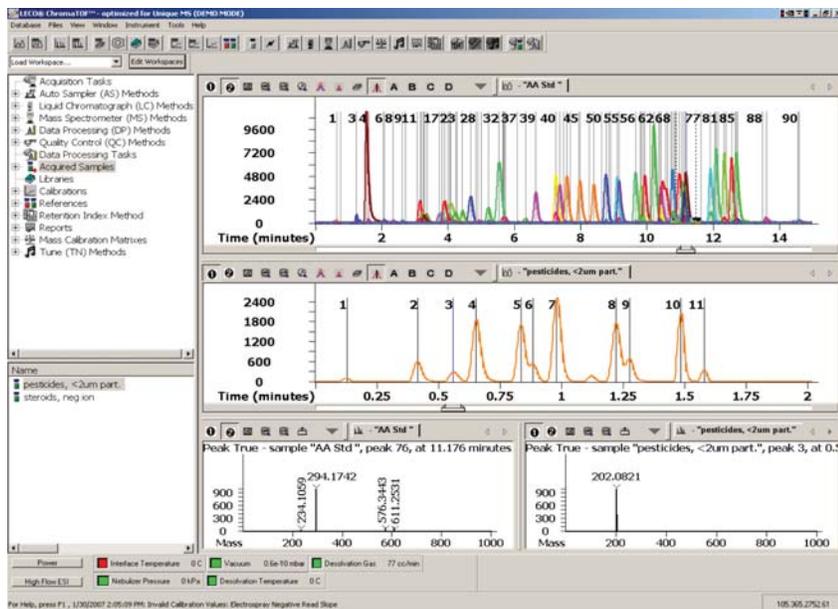


Dynamic Range

Excellent linearity spanning greater than three orders of magnitude can be achieved as shown for the food steroid melengestrol acetate. Mass accuracy coupled with a wide dynamic range provides greater quantitative accuracy and precision with the Unique HT TOFMS.

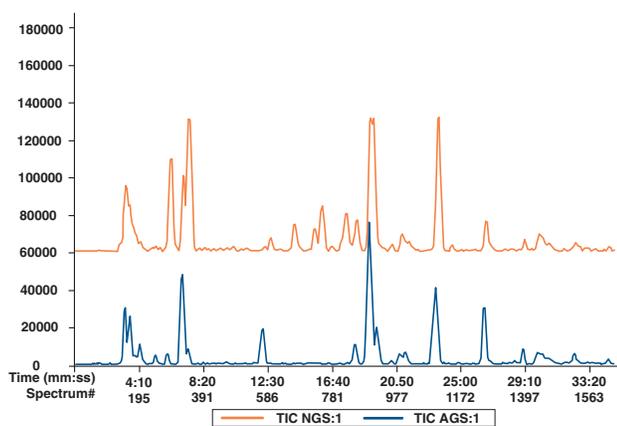
ChromaTOF Software

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.



- Automated Peak Find and True Signal Deconvolution algorithms
- Automated library searching with isotopic pattern comparison, and other industry-leading filtering tools to minimize false hits
- Fully-automated instrument tuning
- Integrated control of the Agilent 1200SL
- Fully-integrated report designer
- Customizable user interface
- Automatically export data in Netcdf, CSV, or Raw file formats

Sample Compare Feature

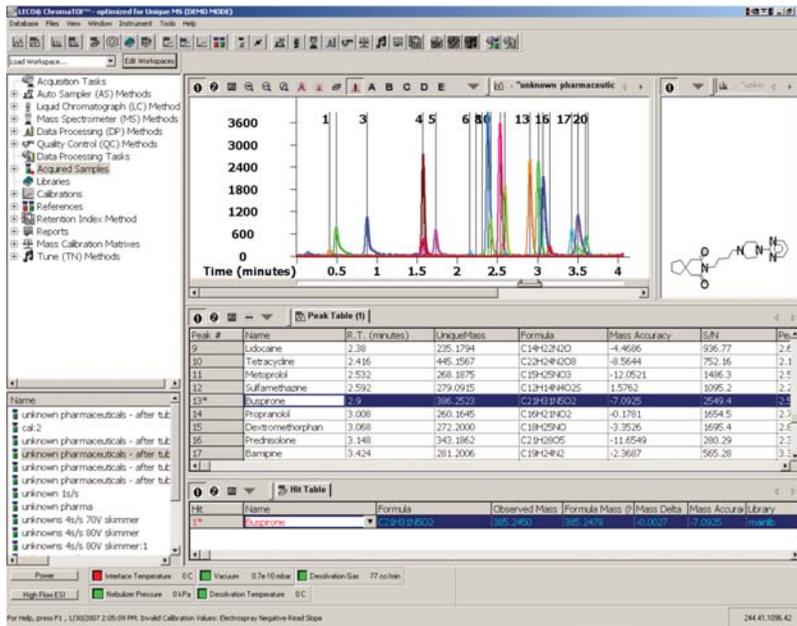


The ChromaTOF Sample Comparison algorithm allows similarities and differences between samples to be rapidly determined. Even differences buried beneath the baseline of the TIC or beneath large matrix interferences can be automatically detected.

Peak #	Name	R.T.	Type	UniqueMass	Concentration Match
1*	Unknown	6:08.32	Unknown	1037.4976	
2	Rd/Gypenoside XVIII	6:58.56	Match	909.5259	116.23 % 822
3	Unknown	7:03.69	Unknown	1031.5081	
4	Rg1	7:20.32	Out of Tolerance	823.4805	294.15 % 951
5	Rg11/Ginseng Root Extract	9:16.64	Not Found	824.4792	
6	Unknown	9:51.36	Unknown	965.4943	
7	Rg1	12:08.32	Unknown	823.4829	
8	Rg12/Ginseng Root Extract		Not Found		
9	Unknown	13:20	Unknown	793.4662	
10	Unknown	17:36	Unknown	1130.5402	
11	Unknown	18:57.92	Unknown	1131.6791	
12	Ra1	19:10.72	Match	1131.6614	6.42 % 879
13	Unknown	19:19.88	Unknown	949.4941	
14	Rb11/Ginseng Root Extract		Not Found		
15	Rb2/Rb3/Rc	19:33.76	Unknown	1103.5777	
16	Unknown	20:59.62	Match	1101.5796	44.63 % 948
17	Unknown	21:09.76	Unknown	1173.5849	
18	Rb2/Rb3/Rc1	21:26.40	Match	1101.5794	192.37 % 888
19	Rd/Gypenoside XVIII	23:24.16	Out of Tolerance	969.5477	3006.21 % 891
20	Unknown	23:29	Unknown	1037.5384	
21	Rd/Gypenoside XVIII/Ginseng Root Extract		Not Found		
22	Unknown	26:29.76	Out of Tolerance	970.5463	207.80 % 1000
23	Unknown	26:50.24	Unknown	940.5307	
24	Unknown	26:59.20	Unknown	1037.6724	
25	Unknown	28:30.08	Unknown	1256.6666	
26	Rg3/Rg2	29:02.00	Match	807.4977	138.13 % 999
27	Rg3/Rg21/Ginseng Root Extract		Not Found		
28	Unknown	29:34.00	Unknown	1358.6139	

Sample comparison results are easily characterized as one of the following: sample impurities, not founds, analytes out of tolerance, or analytes found to be the same between two samples. The results for the comparison of Ginseng extract is shown above.

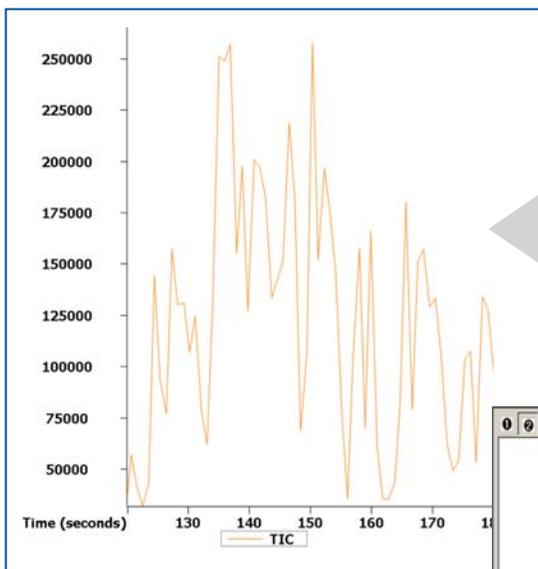
ChromaTOF® Software



Automated Analyte Assignment

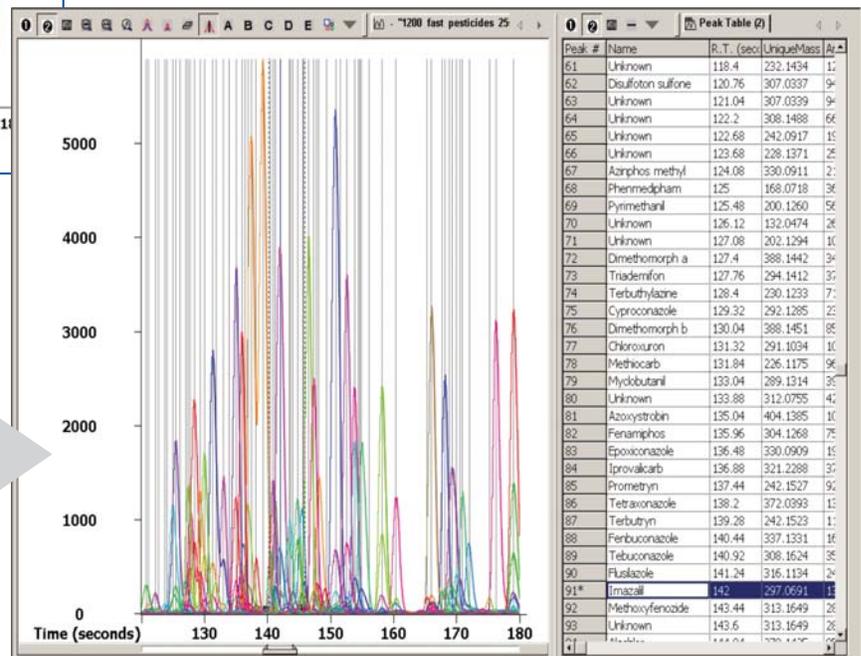
Peak identification has been simplified in ChromaTOF by the addition of an automated library search of commercial and user-created libraries and updated formula calculator tools. By combining accurate mass data with isotopic similarity and additional filters, unrealistic library search and formula results are minimized, and analyte confidence is greatly improved.

- Easy-to-use spreadsheet format simplifies mass axis calibration for accurate mass assignment
- Even peaks with adduct ions or fragment ions as the major spectral feature can be deconvoluted to neutral masses for library searching
- Once the library search is complete, the hit information is automatically imported into the peak table



Others leave you here

Unique HT TOFMS
Delivering the Right Results



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-TOFMS

- 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



Pegasus HT TOFMS

- Acquisition speed up to 500 spectra/second offers you the ideal MS detector for unparalleled throughput
- Powerful Windows®-based ChromaTOF software simplifies component identification—providing a significant increase in efficiency and productivity
- Key features include automated data mining, chromatogram locking, reverse-library search mode, and data-dependent user-defined QC method development
- Ability to upgrade to Pegasus 4D GCxGC



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



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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