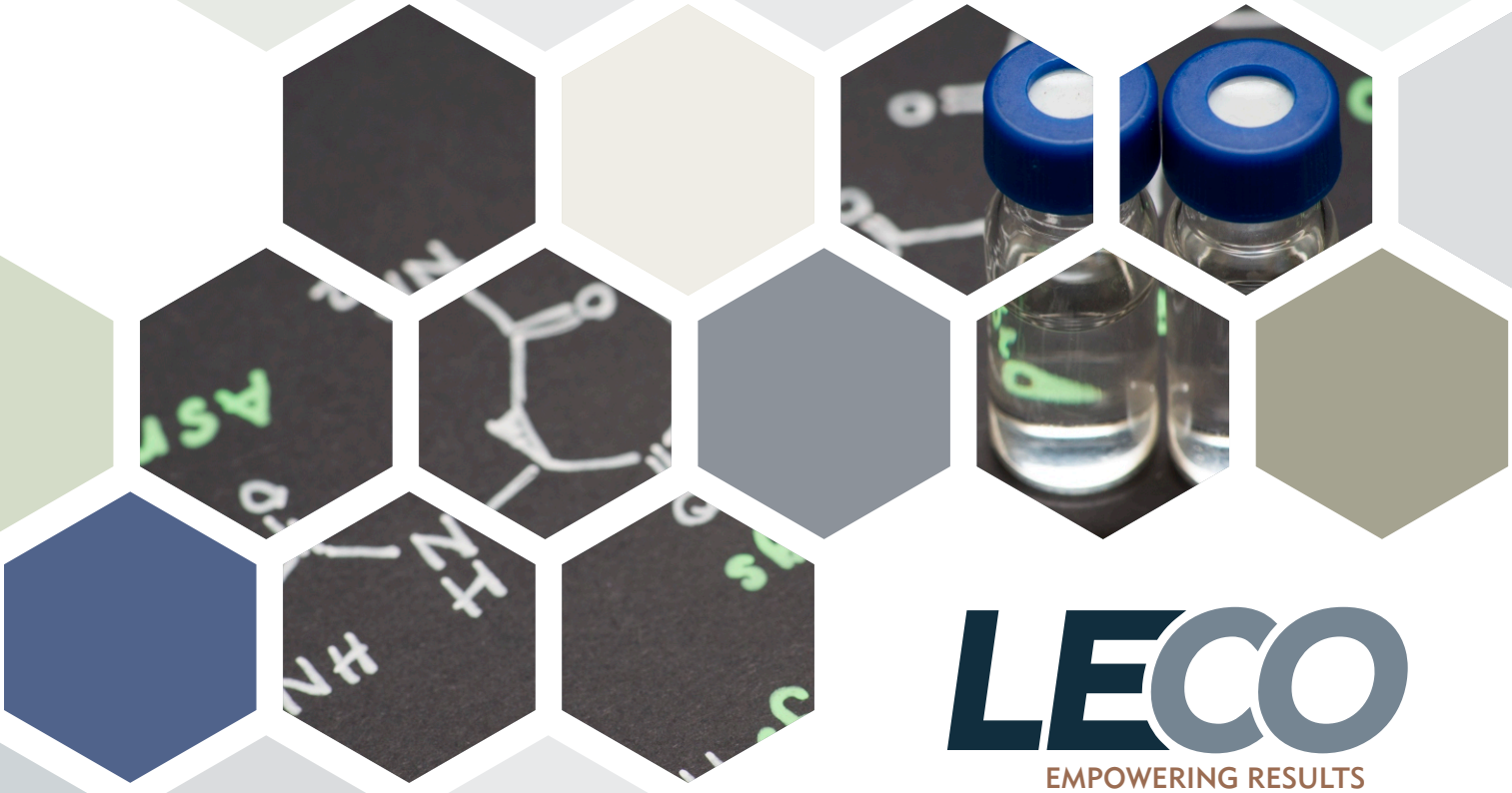
Solutions for
Metabolomics Analysis



LECO

EMPOWERING RESULTS

The Established Leader in GC-MS Metabolomics

Metabolomics presents challenges for both the analytical methods used and the data reduction required to interpret the results. No single analytical technique can be used for complete characterization of the metabolome, and no metabolome has been completely characterized. However, GC-MS provides an established method to analyze the primary metabolome, whereas LC investigates the secondary and tertiary metabolites.

As the established leader in GC-MS metabolomics[1-4], LECO products deliver the accuracy, resolving power, deconvolution, and speed to characterize the most complex biological systems. Our instrumentation has been validated by the industry's most demanding researchers. These attributes are embodied in the following LECO products.

Pegasus® BTX GC-TOFMS

The tried-and-tested reliability and durability of our Pegasus brand in a convenient benchtop unit. Industry-leading sensitivity helps you find and quantify an unlimited number of analytes.

Pegasus BTX 4D GCxGC-TOFMS

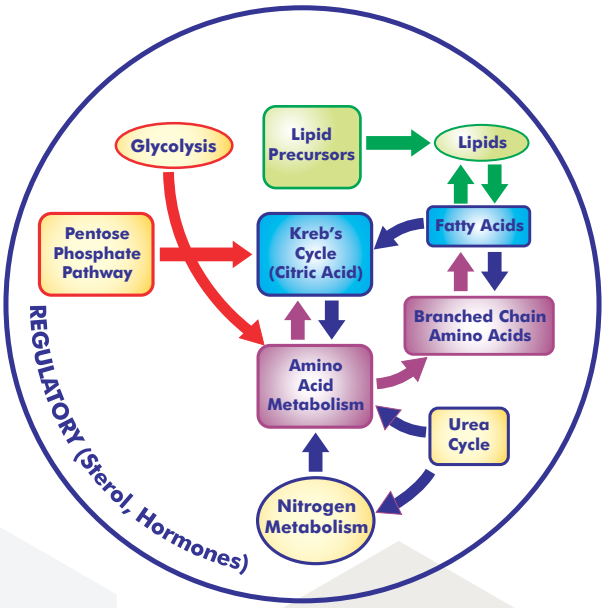
Provides enhanced sensitivity by coupling our benchtop Pegasus BTX with our high performance GCxGC thermal modulation system. This combination provides the ability to interrogate challenging metabolomics samples where the best sensitivity is needed.

Pegasus GC-HRT+
Pegasus GC-HRT+ 4D

GC-MS with industry-leading sensitivity, mass accuracy, and chromatographic resolution leading to identification of more metabolites than ever before.

Our GC-MS Advantage

Our key advantage is the ability to identify and discover more metabolites than other similar technologies. Our speed of full-scan acquisition is unrivaled, and when combined with the power of LECO's ChromaTOF® brand software Deconvolution algorithm, allows an unprecedented characterization of the biological systems under study.



What else is in your samples?

Do you know what you don't know? What is hiding under that chromatographic peak? What are you not observing in your samples today? One of the principal handicaps of metabolomics is detection and identification of unknowns. LECO's GC-MS products give you a distinct advantage to investigate samples and identify components.

Large metabolomic centers leverage GC-MS for the quantitative and qualititative analysis of primary metabolites as well as key precursors to secondary metabolism. Thanks to superior chromatographic performance, GC enables separation of even structurally similar analytes and isomeric metabolites such as fatty acids, which can prove time-consuming to separate by HPLC.

GC-MS and LCMS together provide complementary coverage of a metabolome. For this reason alone, if you're not using GC-MS today, then you could certainly be missing great opportunities of discovery or spending excessive time and effort using the wrong technique. ***Allow yourself to see the complete picture with metabolomics solutions from LECO.***

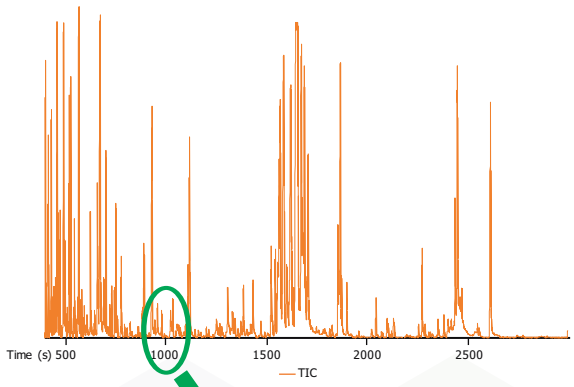
Pegasus BTX GC-TOFMS

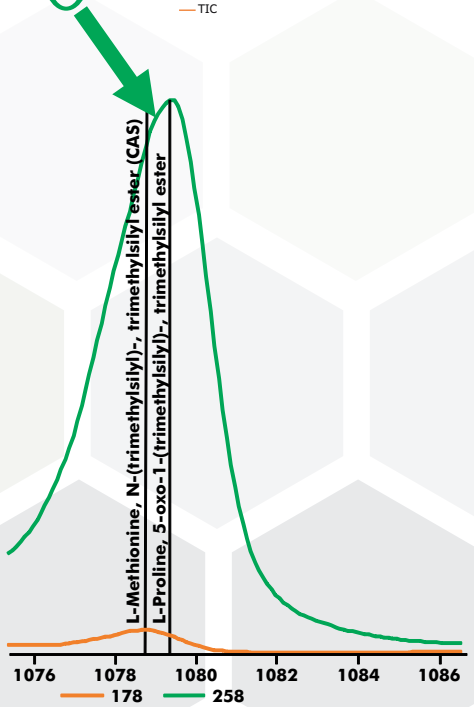
A proven quantitative and qualitative workhorse, the *Pegasus* BTX GC-TOFMS is a staple of leading metabolomics laboratories. The high sensitivity, peak capacity, and reproducibility of GC combined with Time-of-Flight Mass Spectrometry (TOFMS), provides benefits such as reduced analysis times, industry-leading peak deconvolution, and an ability to re-interrogate rich data sets repeatedly for biological inference.

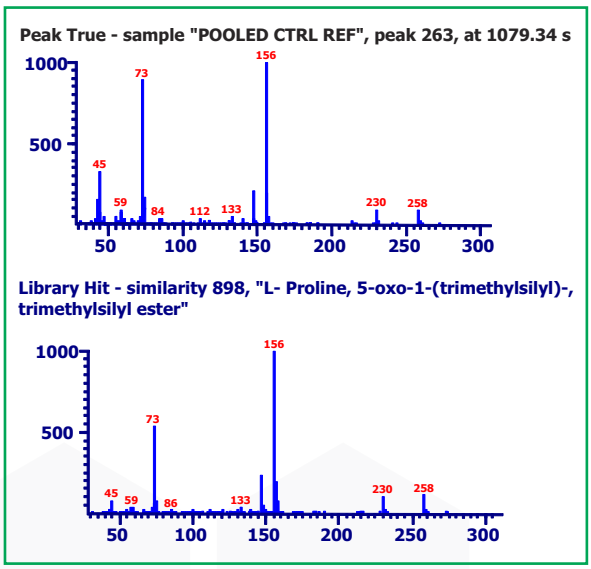
LECO's innovative StayClean® Ion Source design virtually eliminates the need to clean your source—lowering downtime and enhancing productivity.

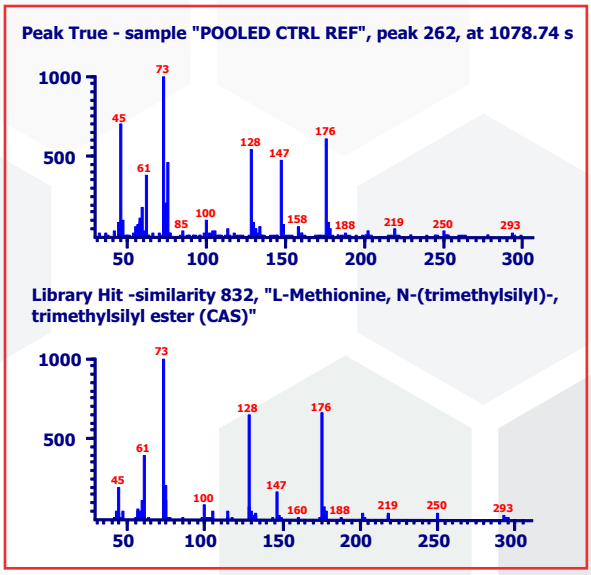
Furthermore, the metabolomics community has built protocols on the *Pegasus* which are peer-reviewed, widely-recognized, time-honored, and with proven results.[1-4]

Winning the Fight Against Coelution







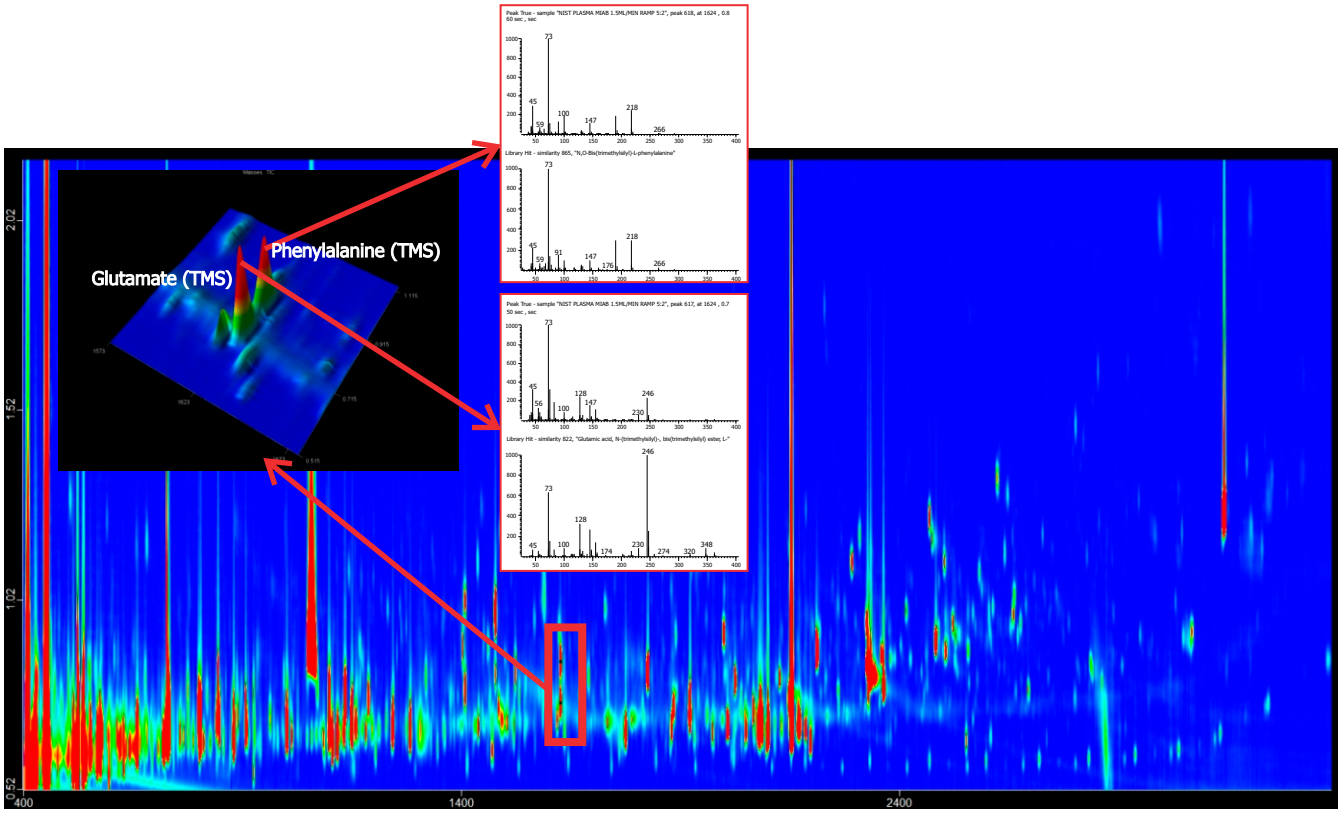


A pair of highly coeluting analytes at significantly different relative abundances are separated easily into their component spectra using True Signal Deconvolution® (TSD®). This example is a TMS-derivatized mouse liver extract, a highly complex sample. LECO's rugged *TSD* algorithm has removed the frustration of poor spectral library matches. *ChromaTOF* was able to deconvolve the two compounds and provide library match scores greater than 830 (83% probability of match). Proline dominates the raw data, yet methionine is completely resolved and identified. These distinct biochemically-important components are present in vastly different concentrations, which would typically be lost in most competitive technologies.

When combined with metabolite-specific libraries, such as the LECO/Fiehn metabolomics library, *TSD* provides scientists with far superior insight into biological content, thus generating superior understanding of experimental variation.

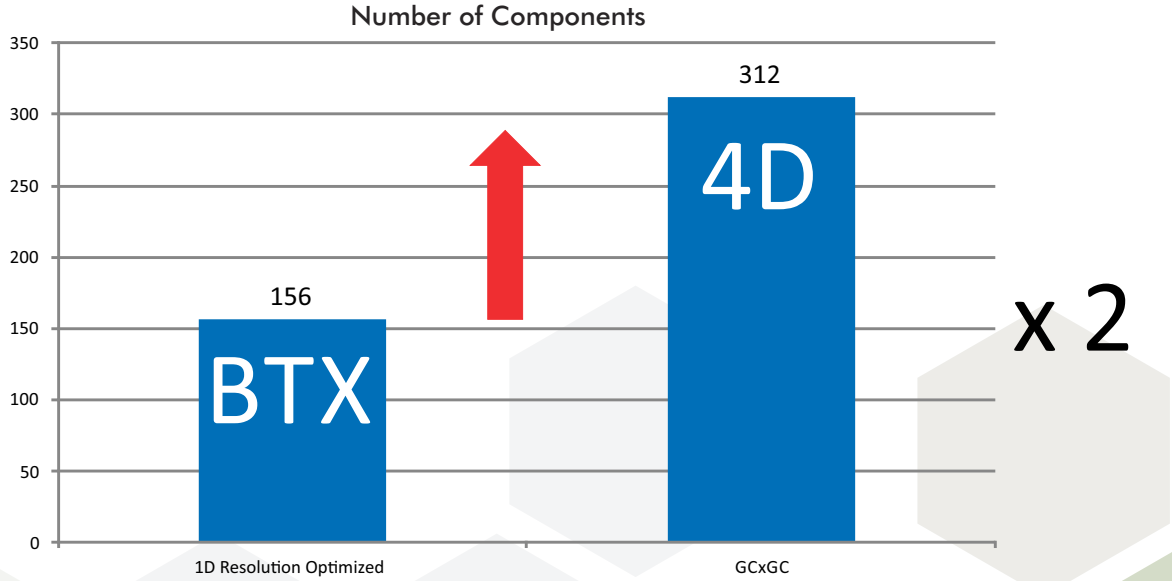
Pegasus BTX 4D GCxGC-TOFMS: See What Else is in Your Sample

The complexity of biological samples often presents one of the biggest challenges to increasing our knowledge. Having the availability of increased separation space allows the scientist to unlock more information from the samples without the possible bias and time investment of additional sample preparation. A pioneer in comprehensive two-dimensional gas chromatography, LECO empowers metabolomics researchers worldwide looking for answers to the question, "What else is in my sample?" The example below shows how the second dimension of chromatography separates 1D coelution very clearly. **GCxGC makes it easy to see what else is in your sample.**



GCxGC allows the user to get to the correct identification of analytes rather than tracking a single mismatched analyte. ***Build your confidence with GCxGC.***

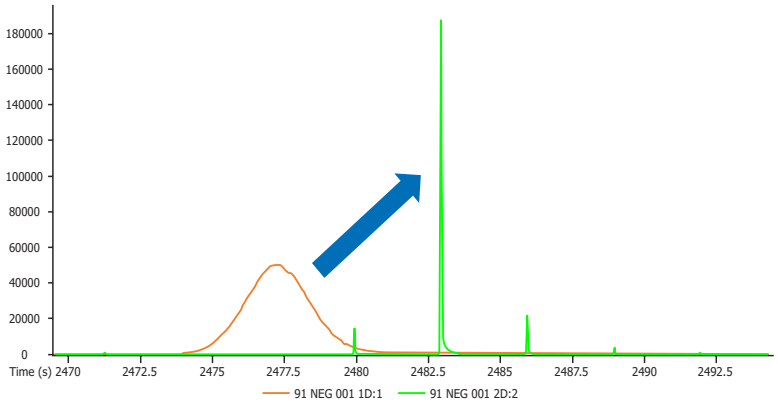
Increased Metabolite Detection and Identification



GCxGC-TOFMS routinely provides more than 2X the number of detected analytes compared to single dimension analyses. In our experiment below we found robustly twice the features with the 4D system as compared to the HT on a plasma extract.

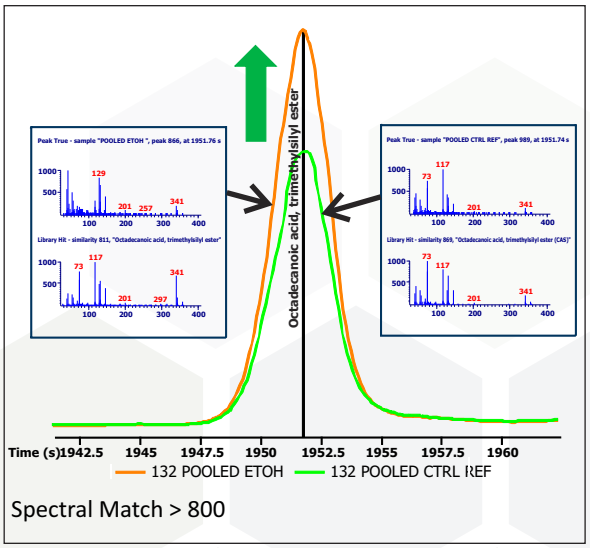
GCxGC-TOFMS Sensitivity Advantage

In addition to the increased identification capabilities and peak capacity, cryogenic focusing occurs at the modulator to sharpen the peaks prior to detection with MS. This enhanced peak detectability is illustrated with arachidonic acid, trimethylsilyl ester, shown below in overlaid one-dimensional and two-dimensional data. Less abundant analytes are enhanced significantly, typically analytes which are below the detection limit with one-dimensional chromatography. These benefits combine to offer a more complete picture of a sample relative to GC alone.

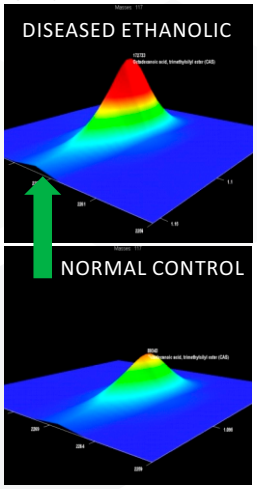


Parameter	GC	GCxGC	Net
Similarity	836	842	Proven Deconvolution
Peak Width	2.57 s	45 ms	x 50
Quant S/N	823	5133	**x 6**

Robust Differential Analysis



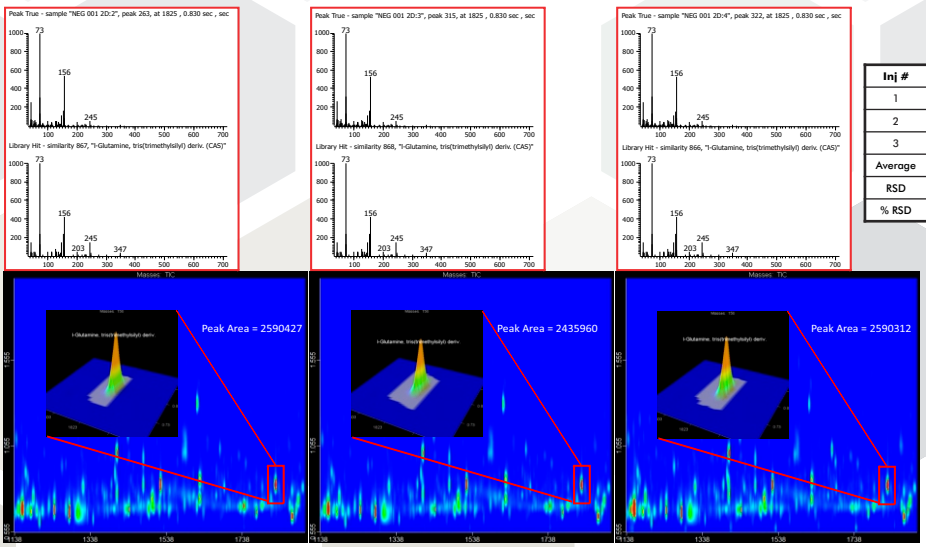
Octadecanoic Acid in Mouse Liver extracts–arrow indicates up regulation



It has been repeatedly proven in academic literature that both deconvolution and GCxGC are quantitatively robust.[9] For instance, in this example of ethanol-treated mouse liver (extract), we see a two-fold relative difference to the normal control octadecanoic peak.

Second Dimension Separation Utility

GCxGC-TOFMS is shown to be reproducible and thus quantifiable in this example of triplicate injections of the same sample comparing peak areas of silylated glutamine, which produced a % RSD of less than 3.5%.[9]

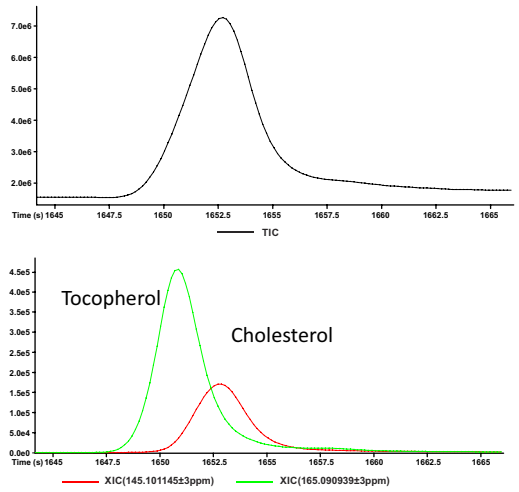


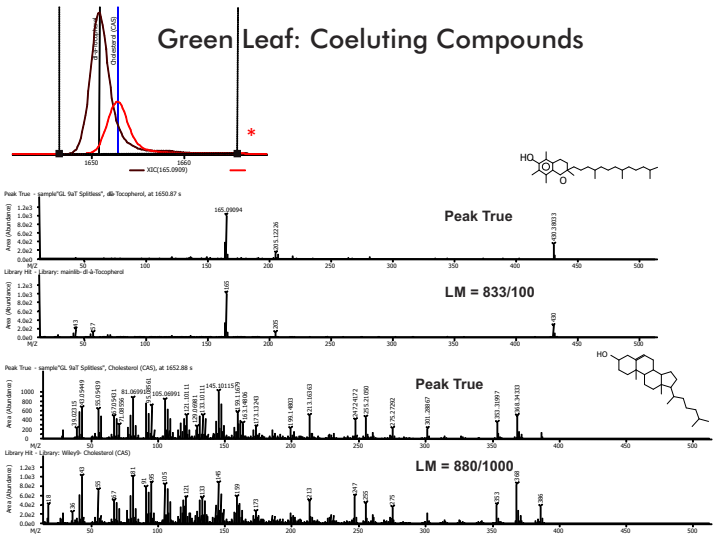
Inj #	Peak Area
1	2590427
2	2435960
3	2590312
Average	2538899.7
RSD	89148.4
% RSD	3.5

High Resolution GC-MS: the Pegasus GC-HRT+

With unknown metabolites presenting one of the most significant challenges to the metabolomics community, having tools to facilitate unknown identification is pivotal to advancing biological studies. High Resolution GC-TOFMS gives you more confidence in identifications and a tool to identify your most challenging unknowns. Our high resolution MS, deconvolution, and novel data acquisition system deliver revolutionary capabilities to the metabolomics marketplace. These capabilities result in mass accuracies which minimize the uncertainty in identification. Accurate mass data reduces the number of potential molecular formula for ions and enables more effective interpretation of mass spectra. Plus, the combination chemical ionization (HR-CI) with electron impact (HR-EI) ionization, which both create accurate mass fragments, provides a proven mechanism for molecular ion identification. This results in more confident interpretation of biochemical pathways, particularly when analytes are differentially expressed.

Proven Deconvolution Using High Resolution TOF

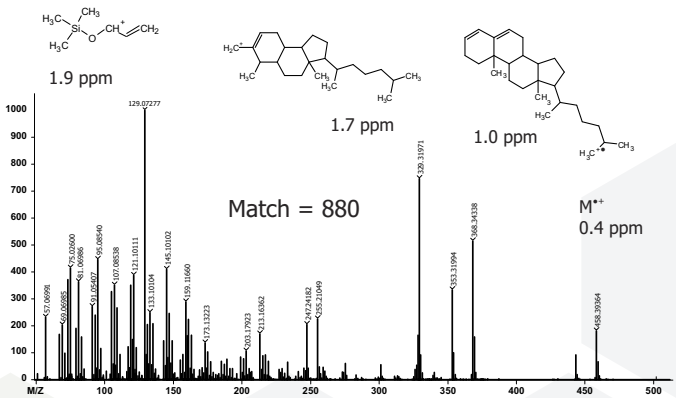




Deconvolution is also a critical component for accurate analysis of complex matrices.[7] An example is provided above for the analysis of analytes in a tobacco leaf extract. Here, two closely-eluting analytes in the sterol region of the chromatogram are shown. The spectra from cholesterol are shown along with that from tocopherol. Accurate spectral deconvolution of the highly complex sterol spectrum due to tocopherol is achieved with two peaks which overlap by more than 70%.

Data Interpretation

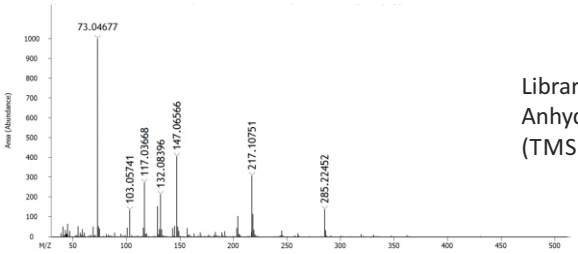
Interpretative Power of Accurate Mass – Cholesterol-TMS (in Rat Plasma Matrix)



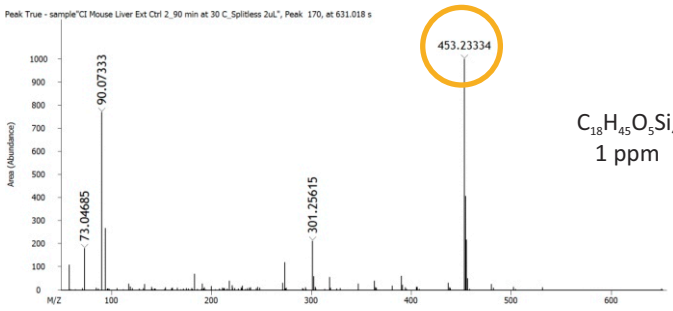
ACD/MS Workbook Suite, version 2012, Advanced Chemistry Development, Inc., Toronto, ON, Canada, www.acdlabs.com, 2014.

HR-EI is a universal ionization type—data-rich with structural information inherent in deconvoluted data (shown here), and has been effectively leveraged for decades. It can be interpreted as a similarity score to a database when the spectra are sufficiently pure, or deconvolved, but leveraging increased mass accuracy can also guide you to what fragments your structure may contain when sufficient library matches are unavailable. In this example of cholesterol-TMS, further interrogation of the spectra quickly reveals confirming fragments of Cholesterol within a very narrow mass accuracy window (<2 ppm). This combined power of deconvolution and accurate mass interpretation give you the tools to truly investigate the "hard stuff." [8]

Confirm Your EI Library Match with Soft Ionization



Library Match 679/1000
Anhydro-sorbitol
(TMS) = $C_{18}H_{44}O_5Si_4$



$C_{18}H_{45}O_5Si_4$
1 ppm

As universal and data rich as HR-EI is, there can still be ambiguity as to molecular ion identification. High Resolution Chemical Ionization (HR-CI) can provide a solution to this problem by delivering a softer ionization mechanism for preservation of the molecular ion, which can then be used to formulate a calculation in its own right, and to filter the possible library hits provided by the EI spectral library search from seven possible identifications to one clear known.

Win the Fight Against Coelution

Pegasus BTX GC-TOFMS | Pegasus BTX 4D GCxGC-TOFMS | Pegasus GC-HRT⁺ 4D

Deconvolution | Sensitivity

GCxGC

Productivity | Reproducibility

Accurate Mass | Structural Interpretation

Identify More with Confidence

LECO products deliver the separation, accuracy, resolving power, deconvolution, and speed to characterize the most complex biological systems.

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LECO's Commitment to Quality and Service

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 life science (metabolomics) industries, we have an instrument configuration to meet your needs.

Technical Research Center

Customer Demonstration and Application Center

Our global network of sales/support includes over 25 subsidiaries worldwide, and is dedicated to customer service and satisfaction. Our commitment to quality is further underscored with ISO-9001:2015 certification. We conform to CE quality and safety specifications, fully testing instruments at our on-site Compliance Testing Center.

LECO Simply GCxGC®

Our *Simply GCxGC* tool takes the worry out of GCxGC by guiding you step-by-step to maximize peak capacity. Learn more at https://www.leco.com/simply-gcxgc

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