
# PEGASUS® GC-HRT

LECO®
Delivering the Right Results

# LECO's Pegasus GC-HRT

## The Ultimate Analytical Instrument


*For complete patent information, see specification sheet 209-212-001.*

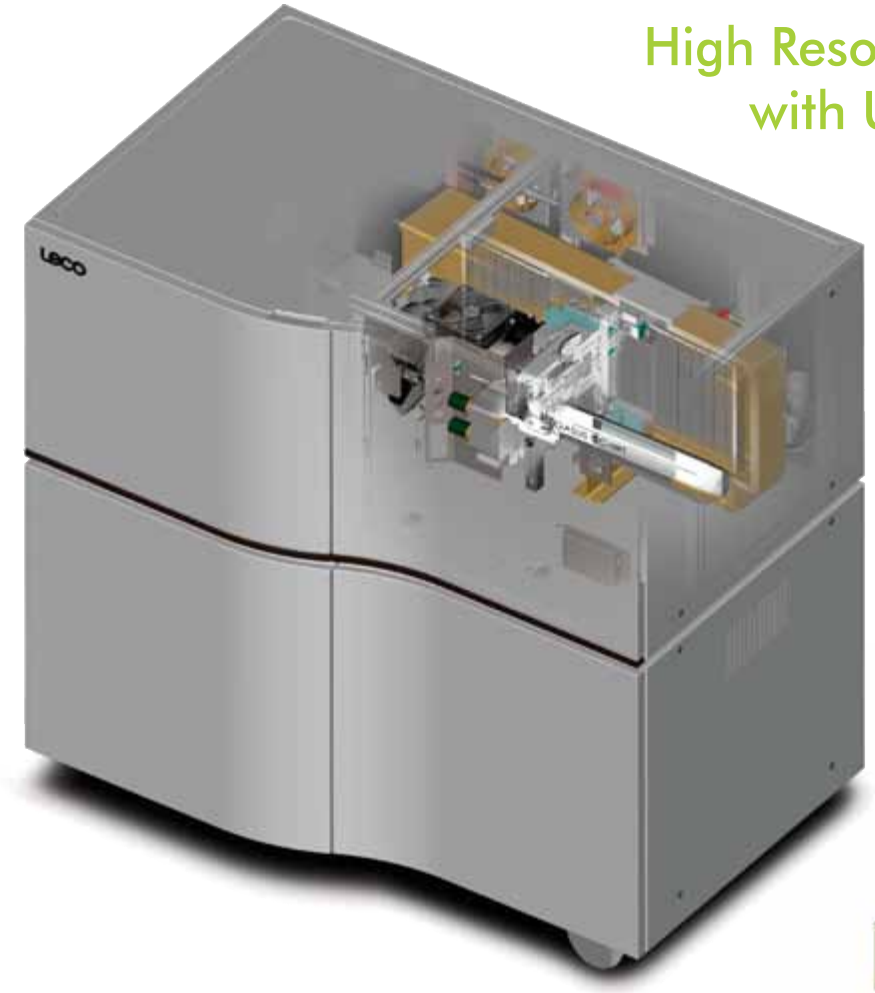
# The No-Compromises Approach to GC-TOFMS

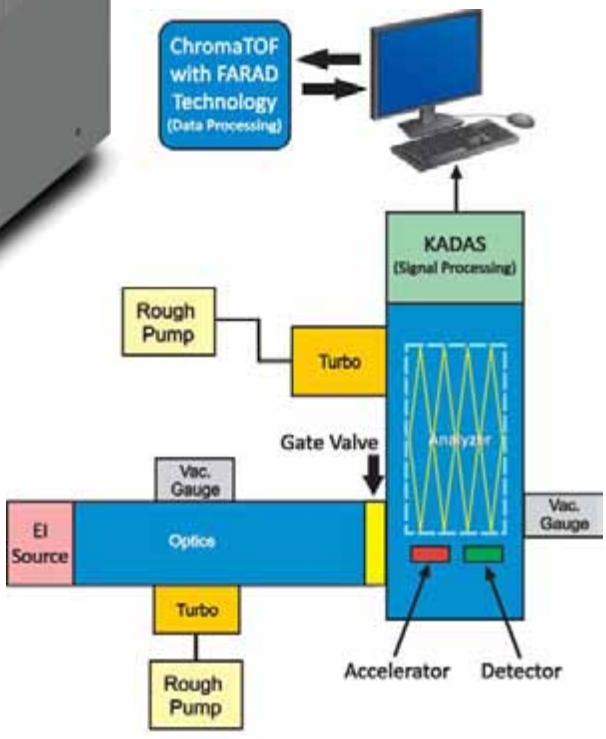
Developed to withstand the rigor of modern analytical demands, the Pegasus GC-HRT provides high-performance MS capabilities, including acquisition speed, mass accuracy, superior relative isotopic abundance, mass resolution, and dynamic range, all available simultaneously—*No Compromises*.

LECO's own Folded Flight Path™ (FFP)™ technology enables resolution of 50,000 FWHM, mass accuracies less than 1 ppm, and acquisition rates up to 200 spectra/second—all with high-integrity isotopic abundance measurements to facilitate rich information content and high-confidence analyte identification.

Signal acquisition is achieved using patented KADAS™ technology to provide high-value, high-integrity output under the most demanding acquisition conditions available. These advances in technology are paired with LECO's exclusive ChromaTOF-HRT™ software, which utilizes True Signal Deconvolution® for accurate peak identification.

## High Resolution MS Combined with Ultra Fast Acquisition



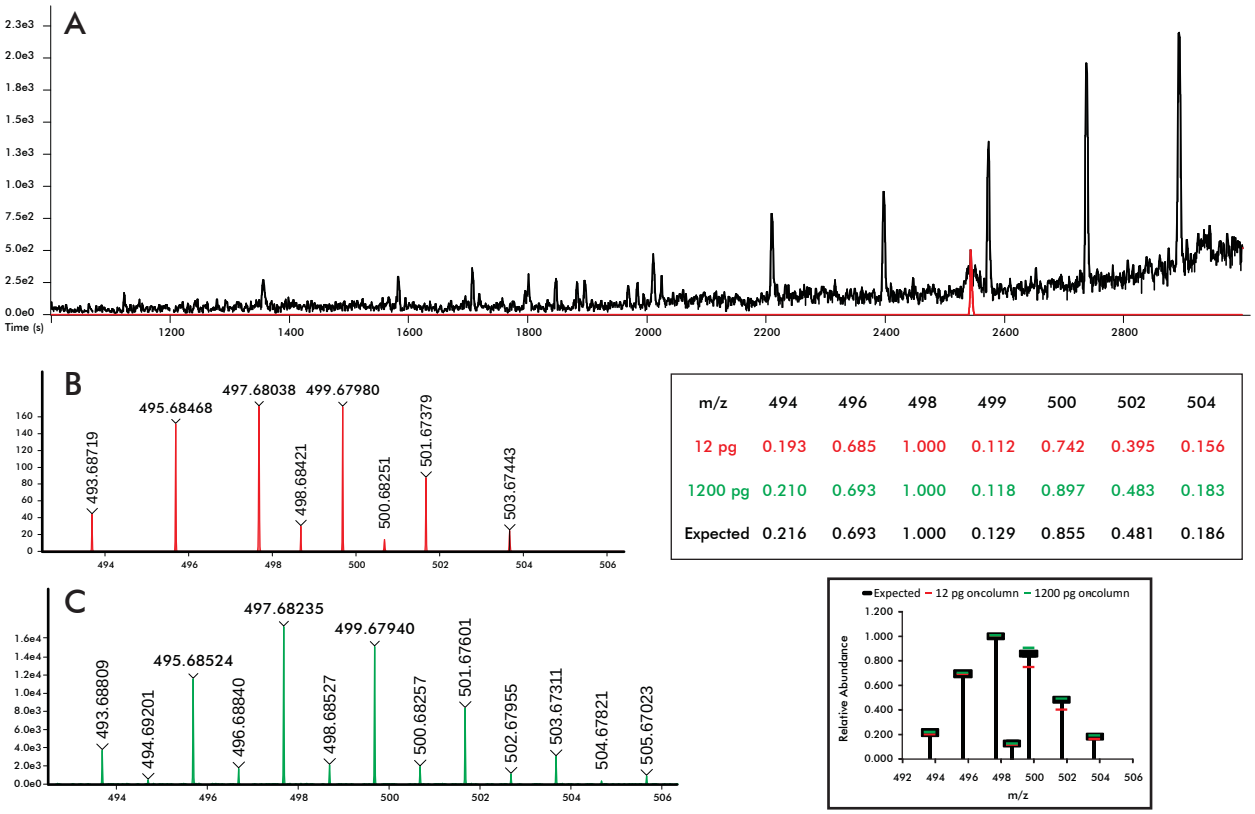

PEGASUS GC-HRT System Diagram

# Industry Leading Resolution

The Pegasus GC-HRT exceeds the performance expectations established for high resolution mass spectrometers, including unsurpassed mass accuracy, resolution, and acquisition speeds—*No Compromises*. As shown in Table 1, high resolution mode resolving power in excess of 25,000 (FWHM) and mass accuracies of <1 ppm are attainable at acquisition rates up to 200 spectra/second. These data show that with the Pegasus GC-HRT, high speed data acquisition does not come at the cost of declining resolution and mass accuracy. These data also show that resolution and mass accuracy are at, or above, the performance specification for the instrument regardless of m/z.

| Acquisition Rate (s/s) | Observed m/z | Expected m/z | Mass Accuracy (ppm) | Resolution (FWHM) |
|---|---|---|---|---|
| 5, 15, 50, 100, 200 | 68.99465 to 68.99468 | 68.99466 | -0.159 to 0.275 | 25629 to 26209 |
| 5, 15, 50, 100, 200 | 218.98494 to 218.98510 | 218.98508 | -0.639 to 0.091 | 28657 to 29188 |
| 5, 15, 50, 100, 200 | 501.97044 to 501.97095 | 501.97059 | -0.297 to 0.719 | 30528 to 31013 |

Table 1. Impact of Acquisition Rate and m/z on Resolution and Mass Accuracy.




| m/z | 494 | 496 | 498 | 499 | 500 | 502 | 504 |
|---|---|---|---|---|---|---|---|
| 12 pg | 0.193 | 0.685 | 1.000 | 0.112 | 0.742 | 0.395 | 0.156 |
| 1200 pg | 0.210 | 0.693 | 1.000 | 0.118 | 0.897 | 0.483 | 0.183 |
| Expected | 0.216 | 0.693 | 1.000 | 0.129 | 0.855 | 0.481 | 0.186 |

Figure 1. A: XIC of PCB 209 at 12 pg on-column overlaid with base peak ion chromatogram
B: Spectrum of PCB 209 at 12 pg on-column
C: Spectrum of PCB 209 at 1200 pg on-column

Accurate recording of isotopic patterns is critical to confident analyte identification. The wide in-spectrum dynamic range of the GC-HRT allows the rich isotopic signature of decachlorobiphenyl (PCB 209) to be accurately recorded over an extended concentration range, as shown in Figure 1. The high resolving power of the GC-HRT allows the extracted ion chromatogram (XIC) of 12 pg PCB 209 on-column to be drawn with no observable noise (Figure 1A). Even at this low level, the spectrum includes the seven most abundant isotopes at the appropriate relative abundances (Figure 1B). At a concentration 100 times higher, the observed spectrum closely matches the theoretical spectrum (Figure 1C).

# Environmental Applications

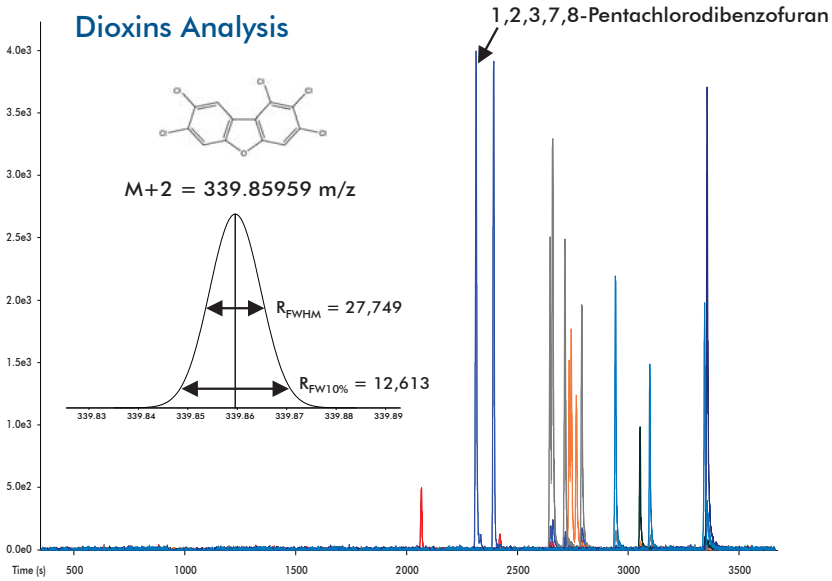



Figure 2. Resolution example for dioxin analyses.

The analysis of dioxins and dioxin-like compounds is of high importance to environmental agencies, as many of these compounds are extremely toxic. Laboratories performing these analyses must adhere to the criteria outlined in EPA method 1613. One of the primary criteria in this method states that the mass spectrometer used be able to achieve a mass spectral resolving power of 10,000 at full width 10%. This criteria is easily achieved in high resolution mode on the Pegasus GC-HRT. Figure 2 shows the extracted ion chromatogram (XIC) for a series of dioxins and furans, with specific attention being drawn to the analyte 1,2,3,7,8-Pentachlorodibenzofuran. The inset displays the mass spectral resolution of the Pegasus HRT for m/z 339.85959 at both full width half maximum and at full width 10% . The resolving powers shown were obtained with the Pegasus HRT operating in high resolution mode. This example highlights the system's ability to meet the resolution criteria set forth by EPA Method 1613 for the analysis of dioxins and furans.

# Comprehensive POPs Analysis

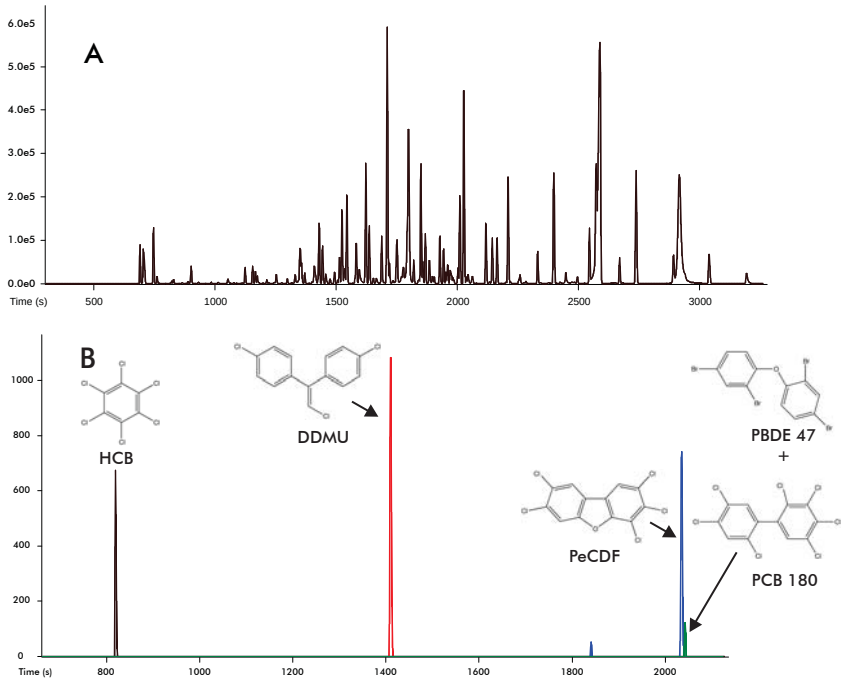



Figure 3: AIC for fish tissue sample (A) and an XIC of the data demonstrating the capability of the GC-HRT to target different for different classes of POPs in a single acquisition (B).

Figure 3 shows the analytical ion chromatogram (A) for a fish tissue sample with elevated levels of polychlorinated biphenyls (PCBs). The targeted PCBs can be easily extracted from the data, but more importantly, additional persistent organic pollutants (POPs) can be analyzed in a single acquisition (B). This demonstrates the utility of LECO's GC-HRT for comprehensive POPs analysis.

# Metabolomics

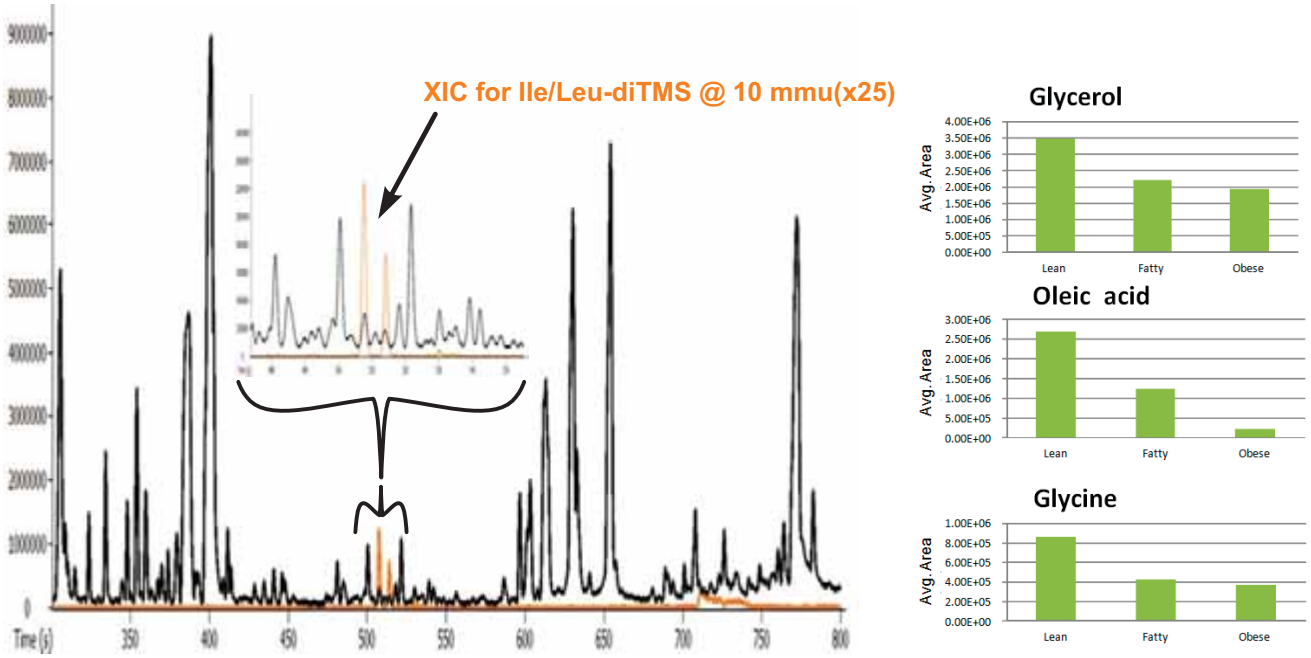



Figure 4. Metabolomics example showing leucine and isoleucine in complex matrix.

The Pegasus GC-HRT provides an ideal platform for discovery analysis, which is used most routinely in metabolomics analysis. The mass accuracy and resolving power provide the ability to selectively extract analyte signal (see Figure 4). This example shows the signals for the TMS derivatives of leucine and isoleucine in the complex background of derivatized plasma. The 25x multiplied signal provides a clear demonstration of the utility of signal extraction using a 10 mmu window. In addition to selectivity, the accurate m/z signal can be quantified and—in the case of lean, fat, and obese rats—provide for the identification of clear and substantial differences in plasma levels of glycerol, oleic acid, and glycine between the phenotypes.

# Pharmaceuticals

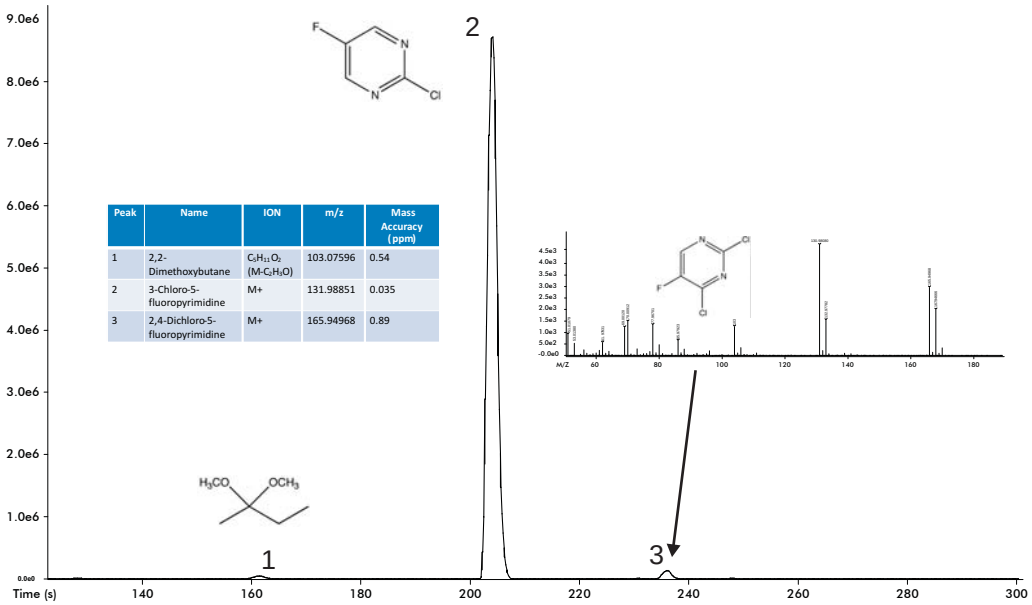
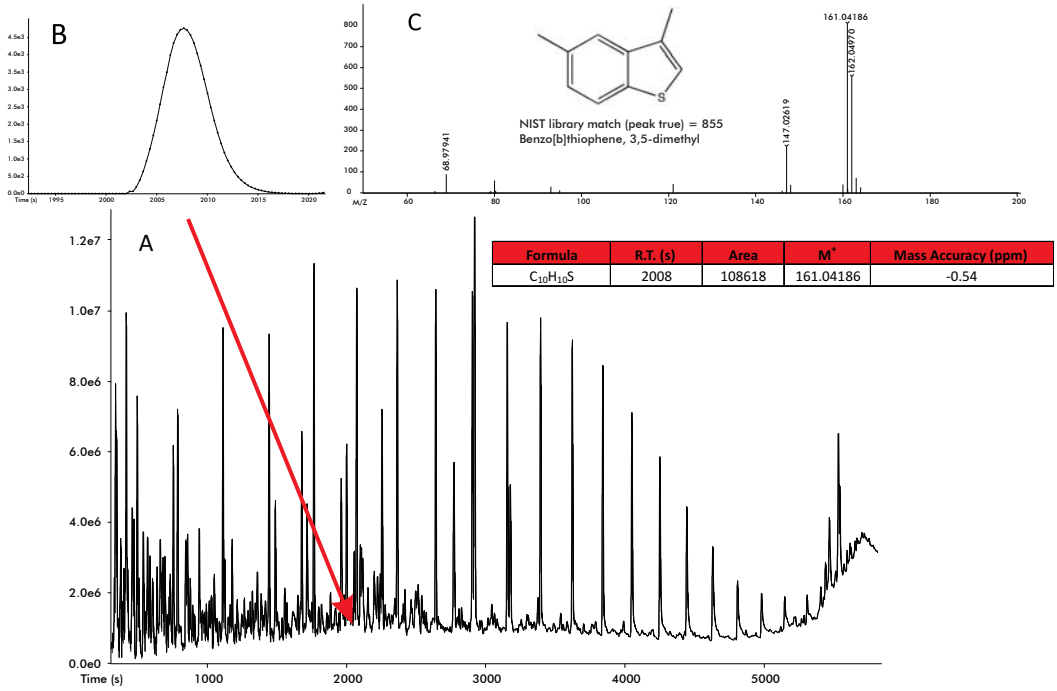



Figure 5. Identification of pharmaceutical process impurities.

The ability to detect and unequivocally identify impurities within a pharmaceutical process is of utmost importance to the pharmaceutical industry. The Pegasus GC-HRT analytical ion chromatogram (AIC) in Figure 5 shows the analysis of a synthetic reactant which was screened for potential contaminants. In this example, 3-Chloro-5-fluoropyrimidine was analyzed and the impurities 2,2-dimethoxybutane and 2,4-dichloro-5-fluoropyrimidine were detected and identified using the NIST mass spectral search database. In addition, accurate mass measurements were used to further support the NIST mass spectral library matches. Mass accuracies for all three analytes were below 1 ppm.

# Petroleum




| Formula | R.T. (s) | Area | $M^+$ | Mass Accuracy (ppm) |
|---|---|---|---|---|
| $C_{10}H_{10}S$ | 2008 | 108618 | 161.04186 | -0.54 |

Figure 6: TIC for Nigerian light oil (A), XIC (B), and mass spectrum (C) of 3,5-dimethylbenzo[b]thiophene.

Sulfur-containing compounds are of particular interest to the petroleum industry. Their levels need to be monitored carefully, since they can have several adverse effects, including poisoning of the noble metal catalysts that are used to increase the octane rating of the naphtha streams, even at extremely low concentrations, and they also lead to increased sulfur dioxide emissions during the burning of the finished fuel product. Figure 6 shows a total ion chromatogram (TIC) from a sample of Nigerian Light Crude Oil and an extracted ion chromatogram (XIC) of m/z 162.0498 for 3,5-dimethyl-benzo[b]thiophene. Also shown is the deconvoluted mass spectrum with a NIST mass spectral library similarity value of 855 out of a possible 1000. The resolving power of the Pegasus HRT in High Resolution mode makes it possible to extract ion chromatograms free of interferences even in the most challenging of matrices. This is important for accurate quantitation of these compounds free of bias from interfering matrix.

# Forensics

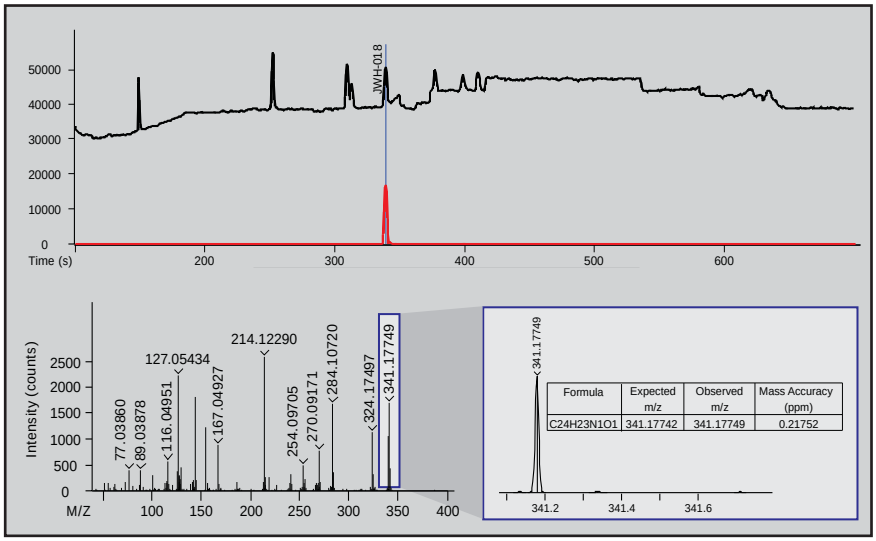



Figure 7. Example of accurate mass measurements used to facilitate formula elucidation of an unknown compound present in synthetic cannabis.

The data shown in Figure 7 provides an example of how accurate mass measurements were used to facilitate formula elucidation of an unknown cannabinomimetic compound. This compound was detected in a synthetic cannabis sample and its spectrum was not present in commercially available mass spectral libraries. Measurements obtained with sub ppm mass accuracy using the Pegasus GC-HRT provided the ability to perform a formula search for 341.17749 m/z. This search, with reasonable constraints, resulted in the correct formula ($C_{24}H_{23}NO$) as the only formula in the hit table. The formula was that of JWH-018, which is a cannabinomimetic compound being used in the preparation of synthetic cannabis.

# Life Sciences and Chemical Analysis Solutions

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, forensics, material science, or metabolomics industries, we have an instrument configuration to meet your needs.

## Citius™ LC-HRT

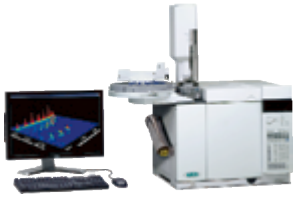
- LC-TOFMS package offers a no-compromise approach to speed, resolution, mass accuracy, isotopic abundance determination, and dynamic range
- Utilizes LECO's Folded Flight Path (FFP) technology to allow users to achieve resolutions of up to 100,000
- Employs ChromaTOF-HRT software with Automated Peak Find and True Signal Deconvolution for seamless data handling
- Versatility of ESI, APCI, and DESI (desorption electrospray) ionization source options, all capable of in-source CID (isCID)

## Pegasus® 4D GCxGC-TOFMS

- Pegasus, with a maximum acquisition rate of 500 spectra/second, offers you the only MS detector optimized for comprehensive two-dimensional GC (GCxGC)
- ChromaTOF software system integrates data acquisition, processing, and reporting tools into one total solution
- The ultimate in chromatographic resolution from the pioneer of GCxGC technology
- Robust, never-clean ion source

## TruTOF® HT TOFMS

- Acquisition speed of up to 80 spectra/second offers you the ideal MS detector for unparalleled throughput
- Powerful ChromaTOF software simplifies component identification—providing a significant increase in efficiency and productivity
- Key features include automated data mining, peak alignment, reverse-library search mode, and data-dependent, user-defined QC method development



## 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) and Electron Capture Detector (ECD)

**Technical Research Center**

**Global Support Center**

**Life Science and Chemical Analysis Centre**

## A Commitment to Quality and Service

LECO instruments are noted 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-9001:2008 certification. We conform to CE quality and safety specifications, fully testing our instruments at our on-site Compliance Testing Center.

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Delivering the Right Results

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