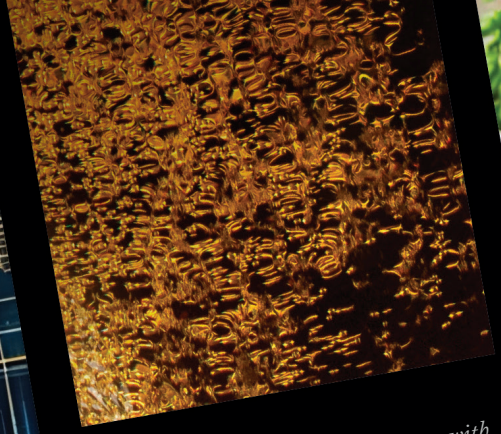
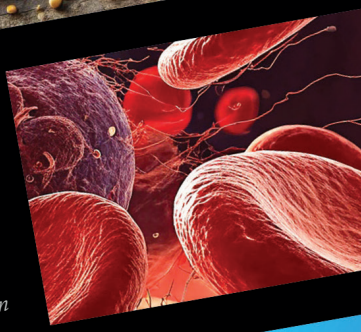
MASS SPEC

From the Analytical Scientist



Mass Spectrometry Supplement 2025

Mass spectrometry is at the forefront of advancing our understanding of human health, environmental science, food quality, and more – powered by pioneering instrumentation and inventive workflows. From real-time flavor profiling to drug detection in the field, this supplement highlights a diverse range of applications that are redefining what's possible with MS technology.



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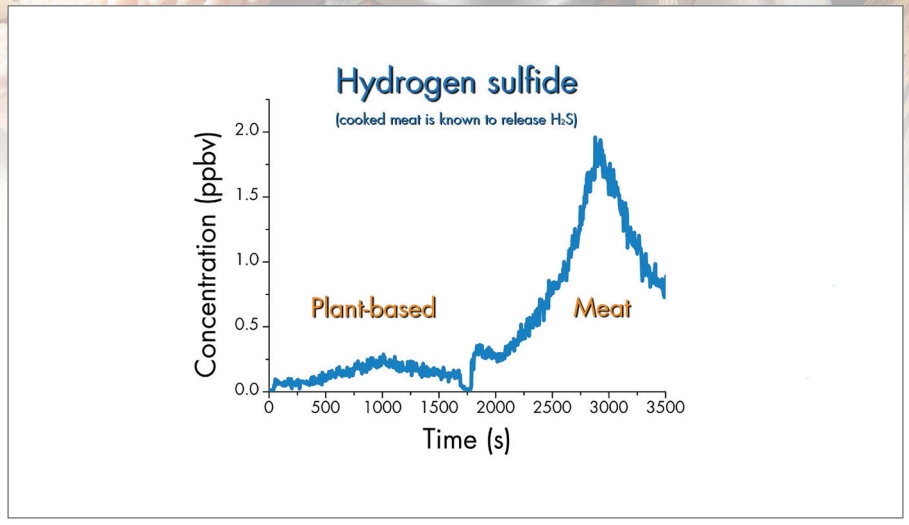
Fake Meat, Real Data: Investigating Sausage Flavors with PTR-MS

A taste of science: insights into food and flavor research in real-time



Proton-transfer-reaction – mass spectrometry (PTR-MS) enhances food and flavor analysis by providing real-time chemical profiling. The IONICON applied science team demonstrated the capabilities of PTR-MS by assessing plant- and meat-based sausages. This investigation revealed distinct differences in their aromatic and chemical composition, demonstrating the potential of PTR-MS in food science applications.

The study began with visual, olfactory, and taste assessments of the sausages, followed by real-time chemical profiling during cooking. PTR-MS enabled the detection and quantification of trace compounds with remarkable precision. In plant-based sausages, the cooking process released flavors dominated by acetic acid and artificial smoke aromas intended to mimic meaty characteristics. Key compounds identified included xylenol, guaiacol, methylguaiacol, and eugenol, which contribute to the smoky flavor. Conversely, meat-based sausages exhibited a distinct profile during cooking, characterized by the release of naturally occurring hydrogen sulfide (H_2S) and other volatile compounds that contribute to their characteristic flavor.

Traditional analytical methods in food science often require extensive sample preparation and laborious workflows. IONICON PTR-TOF instruments offer a transformative alternative with several advantages:

- Direct injection: eliminates the need for sample preparation.
- Real-time quantification: provides immediate results, optimizing workflow efficiency.
- Unmatched sensitivity: detects trace compounds even at very low concentrations.
- High resolution: dissects complex samples with precision, distinguishing isobaric compounds.

This experiment underscores PTR-TOF as an essential tool for modern food and flavor science, capable of quantifying hundreds of compounds with unparalleled accuracy. The ability to analyze and compare the flavor profiles of different food products in real-time opens new avenues for research and development in the food industry.

To read the full application note please scan the QR code now

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Cracking the Code: Machine Learning Unlocks Absolute Quantitation for Cellular Metabolism

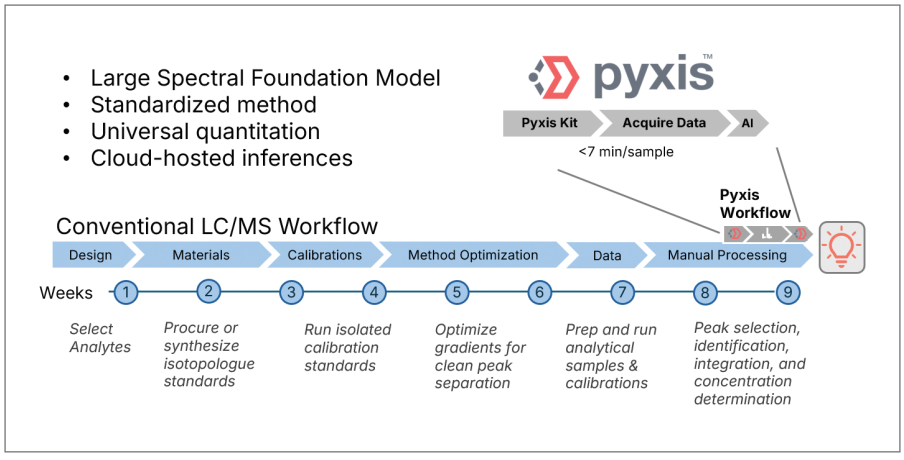


Figure 1. Data acquisition and analysis steps used for both traditional and Pyxis–based absolute metabolite quantitation. Pyxis is built upon our Large Spectral Foundation Model (LSM) and deploys a standardized method and cloud-based software to annotate metabolite identities and absolute concentrations directly from the raw MS data. Pyxis reduces weeks of method development, calibration, and data analysis to minutes.

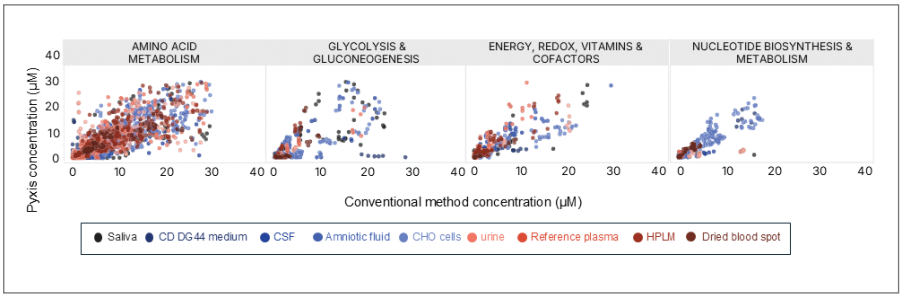


Figure 2. Overview of Pyxis predictions versus conventionally determined analyte concentrations among seven evaluated matrices and four grouped metabolic pathways (an additional five groups are included in the full study, see the link for further details). Sample matrices are colored according to the legend. Pyxis does not need stable-labelled isotopologues to correct for matrix differences.

Traditional approaches to interpreting the complex, unstructured data produced by mass spectrometry (MS) hinder scientific discovery due to their inefficiencies. Utilizing advanced machine learning (ML) to annotate raw MS data represents a transformative shift in data interpretation.

Typical methods for absolute quantification are laborious, expensive, and time-consuming, often requiring eight weeks or more to deliver a biologically actionable result. Following isotopically labeled standard procurement or synthesis, calibration curves must be generated and assessed. Researchers are limited to investigating the biochemical space included in the targeted list of metabolites, prohibiting hypothesis-generating study design and novel discovery.

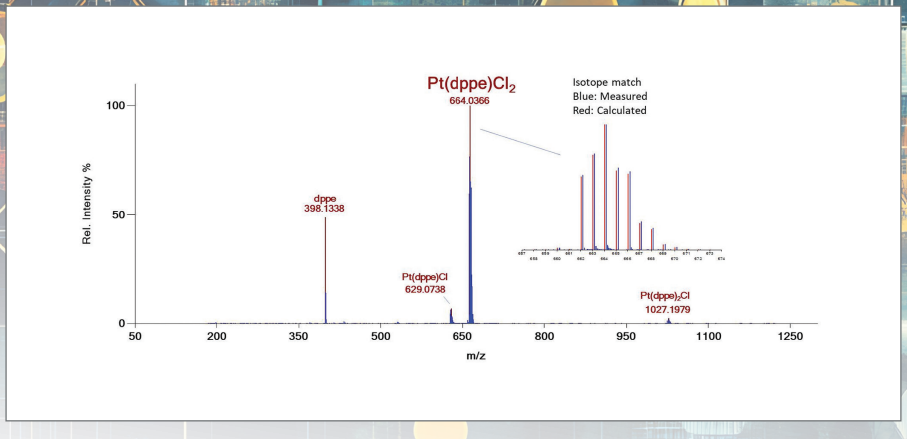
To overcome these limitations, we developed Pyxis (Figure 1).

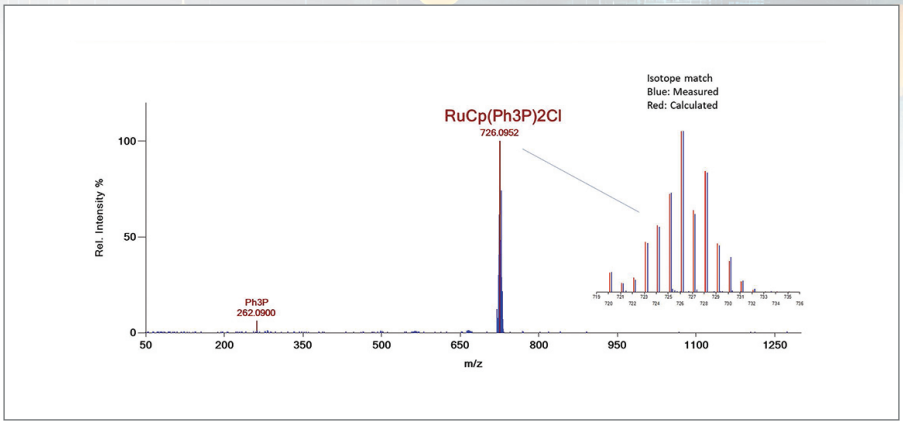
Figure 2 presents a selection of Pyxis-quantified analytes representing multiple major biochemical pathways across central carbon metabolism and beyond. Complete chromatographic resolution is not required; analysis takes under seven minutes per sample. Pyxis exhibited high accuracy in identifying and quantifying metabolites across various metabolic pathways and diverse matrices.

Pyxis condenses days of manual analysis into minutes of automated processing, standardizing compound annotation through ML, and freeing researchers to focus on scientific questions. The underlying LSM and cloud-based platform deliver the predictive power of molecular analysis to scientists across all disciplines and experience levels.

To read the full application note please scan the QR code

Matterworks





Analysis of Organometallic Compounds Using Field Desorption Mass Spectrometry

Soft ionization using Field Desorption yields abundant molecular ions for fragile organometallic complexes

By R.B. Cody F. Fouquet

Field Desorption (FD) is one of the softest ionization techniques available in mass spectrometry and is especially effective for organometallic complexes. This Application Note explores FD using the JEOL AccuTOF™ GC-Alpha with a combination EI/FI/FD ion source. The method is capable of producing dominant molecular ions, even for fragile compounds that commonly fragment under other ionization modes.

In this study, three platinum complexes and one ruthenium complex were analyzed. Each was dissolved in dichloromethane and deposited onto a JEOL 10 µm FD emitter using a precision sampling kit. The emitter was ramped from 0 to 50 mA at 51.2 mA/min, giving an analysis time of 0.98 minutes per compound. Reserpine was used as an internal mass reference, and spectra were acquired over a range of m/z 50–1600 at 1 spectrum per second.

The FD spectra showed molecular ions as the base peaks for all four compounds. Minor peaks related to ligand loss, chloride loss, and sodium adducts were also present. Mass accuracy was high, with differences between measured and calculated m/z values remaining within a few millimass units (mmu).

The results confirm that FD provides reliable and rapid characterization of organometallic complexes, with good isotopic resolution and mass accuracy. This method is especially advantageous for samples that are sensitive to fragmentation. Additionally, a liquid introduction FD ionization (LIFDI) source is available for air-sensitive samples.

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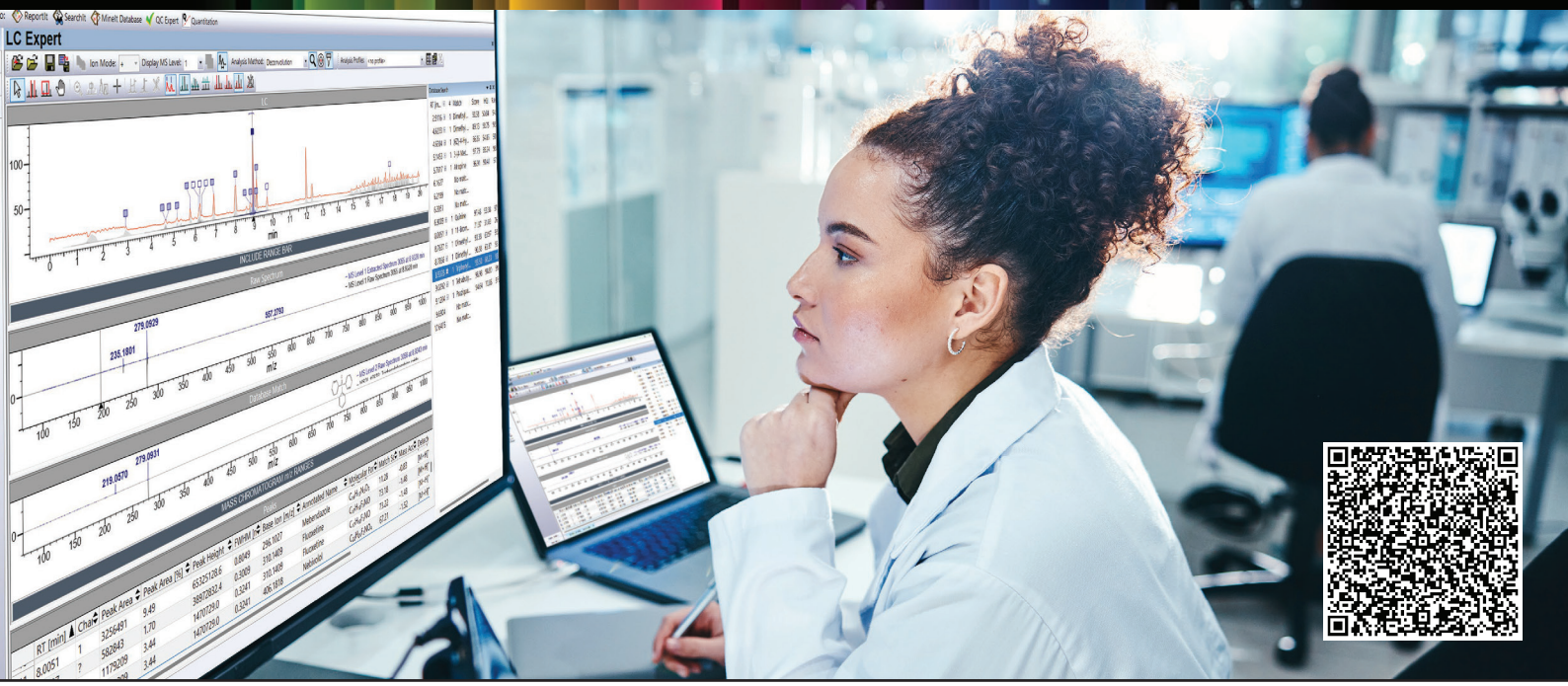

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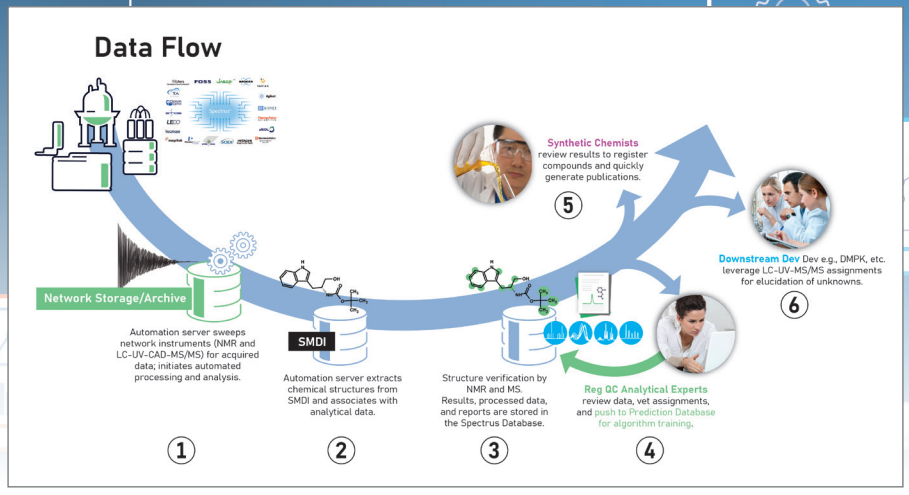
Accelerating Discovery Through Centralized Analytical Data Management

How Genentech is using a unified database to drive efficiency, insight, and collaboration



At Genentech, the Analytical Research team within Discovery Chemistry supports early-stage drug discovery by driving efficient, insightful analytical workflows. Their focus is on rapidly advancing molecules into development, optimizing data use while minimizing material consumption, and leveraging existing data to predict outcomes and reduce experimental burden.

Centralizing knowledge to accelerate tomorrow's breakthroughs

The goal was to create a unified, structure-rich database that accelerates structure elucidation, improves compound tracking, and eliminates data silos. Using ACD/Labs' vendor-neutral Spectrus® Platform, Genentech's workflow automatically captures, processes, and stores diverse analytical data types (e.g., NMR, LC/MS) with associated metadata. This enables searchable, standardized, and accessible data storage – supporting long-term learning, streamlined workflows, and smarter decision-making.

From data to discovery: unlock scale, speed, and scientific insight

Scale and data utilization

The team supports medicinal chemistry by purifying and conducting quality control on thousands of compounds annually, with most bioassay-ready molecules turned around in one day. About 60 compounds per year require deeper analysis for animal studies, taking up to two weeks. Given the data volume and complexity, centralizing and learning from this information is essential for accelerating workflows, enabling data reuse, and improving decision-making across discovery and development.

Accelerated structure elucidation and verification

Once data is in the database, software tools support structure verification (proposed vs. alternative structures), creation of LC/MS purity tables, and generation of reports. This helps accurately identify impurities and ensures a high-confidence link between the experimental data and the chemical structure it represents.

Downstream use and efficiency gains

The database integrates with Genentech's internal Oracle infrastructure for small molecule registration, material tracking, and study progression (i.e., DMPK, biochemical, safety) – supporting downstream teams by enabling rapid dereplication and improving structure elucidation accuracy. High-resolution MS and NMR data can be exported to streamline IP and publication workflows. As compounds move from discovery to development, impurity profiles and spectral data follow for continuity. An ongoing initiative uses confirmed MS/MS data to train machine learning models for improved future structural annotation.

By leveraging the Spectrus Platform, the team has built a robust and scalable infrastructure that streamlines workflows, supports cross-functional collaboration, and advances broader scientific objectives.

Learn more about how Genentech built a database – now and for the future

ACD/Labs

Eliminating Carryover in the Analysis of Alcohol Biomarkers in Whole Blood on Raptor C8 by LC-MS/MS

The method herein provides a robust and accurate analysis of the two most predominant phosphatidylethanol (PEth) homologues in whole blood using a simple protein precipitation

Phosphatidylethanol (PEth) is a group of phospholipids exclusively formed in cell membranes when in the presence of ethanol. As such, these compounds are adequate biomarkers for alcohol use, having a much longer half-life than ethanol in blood, and can be used to distinguish drinking patterns with a window of detection from 2-4 weeks. Among the multiple homologues of these compounds, PEth 16:0/18:1 (palmitic acid/oleic acid-POPEth), is the predominant compound (approximately 37 percent of total PEth) while the second most abundant PEth compound is 16:0/18:2 (palmitic acid/linoleic acid - PLPEth), which accounts for 25 percent.

To read the full application note please scan the QR code now

Table I: Method Conditions

Analytical Column:	Raptor C8 50 x 2.1 mm, 2.7 µm (cat.# 9303A52)		
Guard Column:	Raptor C8 EXP Guard Column Cartridge 5 x 2.1 mm, 2.7 µm (cat.# 9303A0252)		
Injection Volume:	5 µL		
Column Temperature:	30 °C		
Ion Mode:	ESI-		
Mobile Phase A:	Water, 5 mM ammonium acetate		
Mobile Phase B:	Acetonitrile:IPA 90:10		
Gradient:	**Time**	**Flow Rate**	**%B**
	0.00	0.6	70
	2.50	0.6	90
	3.00	0.6	95
	3.01	1.0	95
	3.50	1.0	100
	3.51	0.6	70
	5.00	0.6	70

RESTEK

A Highly Sensitive Method for Quantification of Semaglutide in Human Plasma by LC-MS/MS

Applying robust quantitative methodology to measure a peptide-based drug at low levels in human plasma

By Nitin S. Shukla, Nitish R. Suryawanshi, Samruddha H. Chavan, Devika V. Tupe, Siddhesh Ghadi, Ramesh Manigiri, Jitendra Kelkar, Pratap Rasam

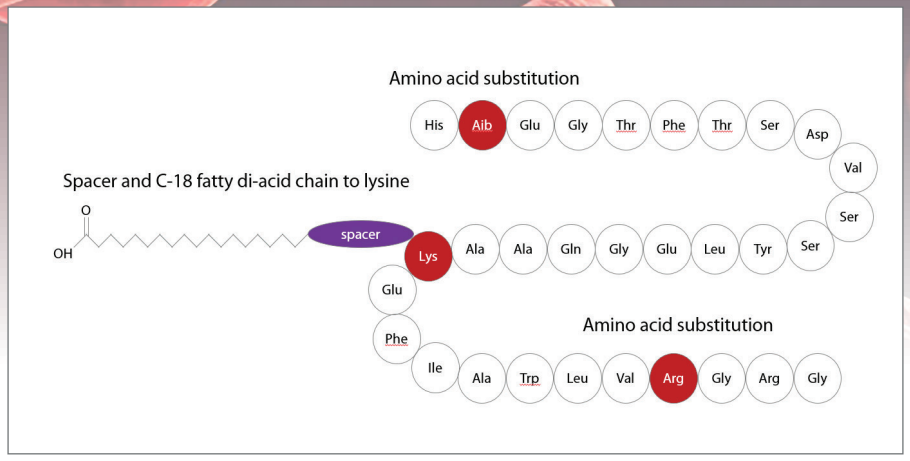


Fig 1. Semaglutide is a modified GLP-1 receptor agonist peptide that enhances glucose-dependent insulin secretion whilst slowing gastric emptying and reducing glucagon secretion in a glucose-dependent manner.

Fig 2. LCMS-8060NX triple quadrupole tandem mass spectrometer.

Semaglutide is a glucagon-like peptide-1 (GLP-1) receptor agonist that was developed for the treatment of type II diabetes, and more recently, it has been applied to the treatment of obesity and shown to reduce the risk of major adverse cardiovascular events. With a 94 percent homology to human GLP-1, semaglutide is a long-acting GLP-1 receptor agonist, with the extended half-life attributed to structural modifications to promote albumin binding and prolonged renal clearance with resistance to metabolic degradation (Fig. 1). Following GLP-1 activation, semaglutide enhances glucose-dependent insulin secretion whilst also slowing gastric emptying and reduces glucagon release. The use of semaglutide, also known under the trade names Ozempic, Wegovy and Rybelsus, has increased markedly over recent years to treat type II diabetes and as a weight loss treatment. However, the misuse of semaglutide by a non-diabetic and non-obese population and by a young public has also grown. There is now a requirement to develop methods to quantify semaglutide and other glucagon-like peptide-1 (GLP-1) analogs to assess the clinical safety and efficacy for new therapeutic analogs but also to monitor for misuse in toxicology screening programs.

To meet both a clinical need to evaluate new therapeutic drug bioavailability and efficacy, and a toxicology need for screening programs to detect misuse, a highly sensitive and selective LC-MS/MS method was developed.

This method targeted semaglutide spiked into human plasma over a calibration range of 0.2–600 ng/mL, with quality control samples at four levels (LLOQ 0.2, LQC 0.6, MQC 200 and HQC 480 ng/mL). Human plasma samples (300 µL) were extracted using protein precipitation followed by SPE to remove phospholipids (Phree, Phenomenex), and semaglutide was quantified applying an external standard method (no internal standard was used in this assay). The targeted component was separated using reverse phase

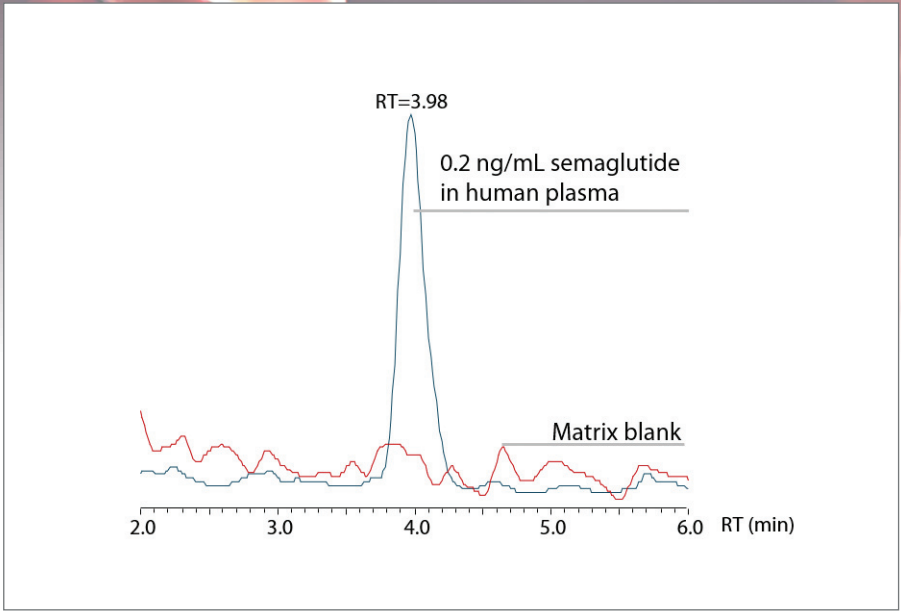


Fig 3. Lower limit of quantitation (LLOQ) at 0.2 ng/mL semaglutide in human plasma highlighting the assay specificity compared to the matrix blank.

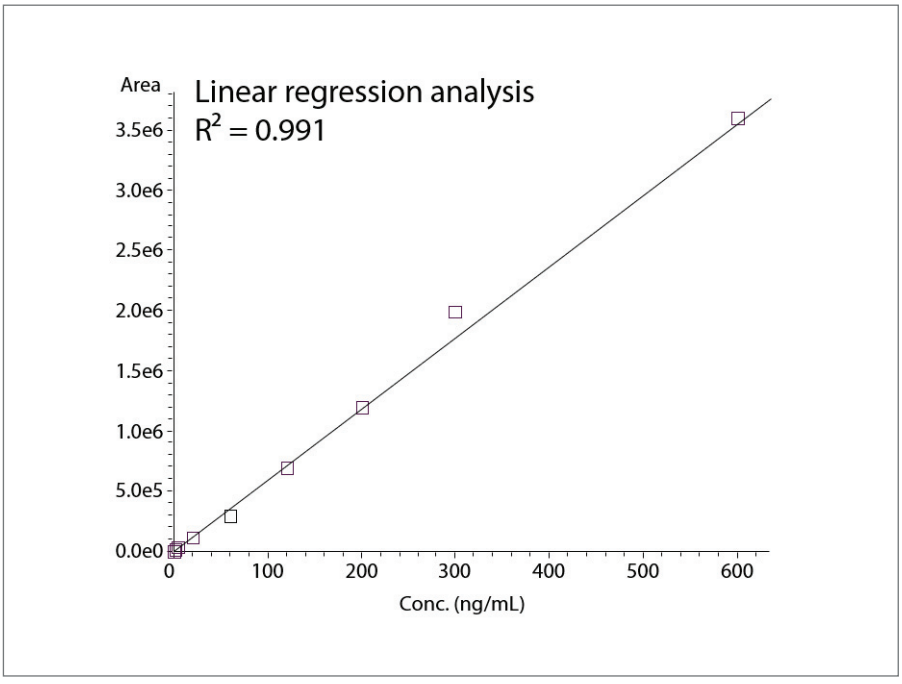


Fig 4. Calibration curve for semaglutide in human plasma between 0.2 to 600 ng/mL highlighting a linear response and a dynamic range over 3 orders of magnitude.

chromatography with a Shim-pack Scepter™ Claris column (C8-120, 3µm, 2.1 x 100 mm) on a Shimadzu Nexera LC system and detected by LC-MS/MS using the Shimadzu LCMS-8060NX high-sensitivity triple quadrupole system.

To optimize component detection, the most abundant charge state was acquired using multiple reaction monitoring (MRM) with a quantifier ion at m/z 1029.20 > 1302.55 and a qualifier ion at m/z 1029.20 > 1359.15, corresponding to the $[M+4H]^{4+}$ ion (semaglutide has a molecular weight of 4113 Da).

The method resulted in a linear calibration curve over the concentration range studied (coefficient of determination (r^2) > 0.99), showing an accuracy within 85–115 percent for all samples, precision for QC samples better than 15 percent and a linear dynamic range with over 3 orders of magnitude. At the lower limit of quantitation (LLOQ) of 0.2 ng/mL, no matrix interference or target component carryover were observed. Assay specificity was confirmed by comparing the matrix blank to the LLOQ of 0.2 ng/mL (signal-to-noise ratio for the 0.2 ng/mL was 5:1), with a percentage coefficient of variation of 6.3 percent.

As a bioanalytical assay, the method developed on the Shimadzu LCMS-8060NX triple quadrupole mass spectrometer resulted in a high sensitivity, achieving an LLOQ of 0.2 ng/mL, high accuracy of quantitation and repeatability of the method < 7 percent at the LLOQ without the requirement for an internal standard. With a dynamic range of over three orders of magnitude, the method can be applied to both a clinical need in assessing new therapeutic analogs and a toxicological need in detecting misuse.

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SHIMADZU
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Traditional Belgium Beer Aroma Analysis and Comparison

Enhanced GCxGC data processing by ChromaTOF Sync 2D for traditional Belgium beer aroma analysis and comparison

By Lena DuBois

Beer brewing relies on the analysis of volatile compounds to ensure quality and optimize processes. The volatile profile of beer provides valuable insights into raw materials, fermentation, maturation, and potential defects. This type of aroma analysis often requires advanced analytical techniques and efficient data processing workflows due to the complexity of such samples. Comprehensive two-dimensional gas chromatography (GCxGC) provides high-quality data, but effective interpretation relies on robust software tools, like LECO's ChromaTOF Sync 2D software.

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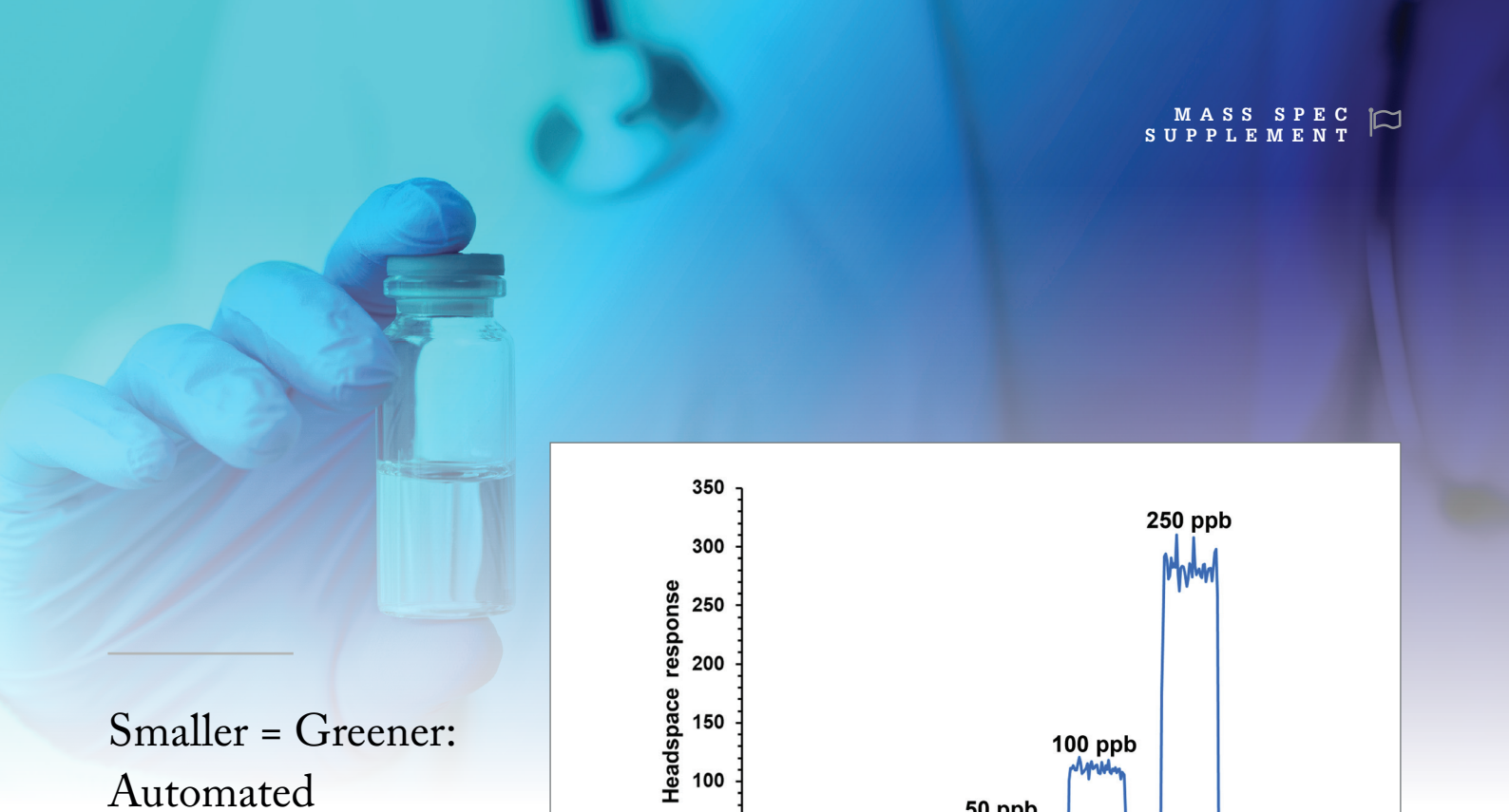

Smaller = Greener: Automated Headspace-SIFT-MS Analysis Using 2-mL Sample Vials

By Mark J. Perkins and Vaughan S. Langford

Figure 1. Real-time SIFT-MS analysis of sequential headspace injections (0.5 mL at 10 µL/s) from blanks and four aqueous atoluene standards (as annotated) prepared with 1 mL of solution in 2-mL vials.

Automated headspace-selected ion flow tube mass spectrometry (SIFT-MS) supports a variety of static headspace approaches for sensitive analysis of diverse volatile compounds. To date, 20-mL headspace vials paired with 2.5-mL headspace syringes have primarily been utilized because, with the slow sample injection required for direct SIFT-MS analysis, larger volumes better matched sample inlet flow. However, moving to smaller sample vials is advantageous from a sustainability perspective, since it addresses the green analytical chemistry (GAC) goal of reduced consumable waste (from 17 g per sample to 3 g).

Syft Technologies SIFT-MS instruments are best automated using syringe-injection autosamplers. Conversion from 20-mL (and 10-mL) vials is straightforward, with a change of vial tray, addition of inserts into the incubator/agitator, a software change to the needle guide setting, and a reduction in syringe needle penetration (8 mm instead of about 20 mm). Extracted headspace volumes are necessarily smaller than for 20-mL vials, usually lying in the range 0.5 to 1.0 mL, whereas injection rates into the SIFT-MS instrument are typically slower. When necessary, maximum sensitivity is achieved by using a large phase ratio (β). In practice, this means using as much sample as possible (e.g., 1 mL of solution) and injecting as fast as the SIFT-MS method can accommodate.

Figure 1 shows SIFT-MS analysis, in one continuous acquisition, of a blank and four standard concentrations of toluene in aqueous solution (10, 50, 100, and 250 ppb). The linearity, as measured by the regression coefficient (R_2), was 0.9995. The limit of quantitation (LOQ) under these conditions is estimated at 1 – 2 ppb in solution. Other volatiles have similar performance. Repeatability for volatile compound measurements in aqueous solution and polymer headspace is excellent, with typical relative standard deviations of less than 5 percent.

The use of 2-mL sample vials is feasible for applications such as residual solvents, quantitation of volatile impurities in personal care products, screening of polymers (targeted and untargeted), and rapid identification of microplastics. Sustainability is enhanced due to a reduction of over five-fold in the mass of vial waste and the use of smaller quantities of samples.

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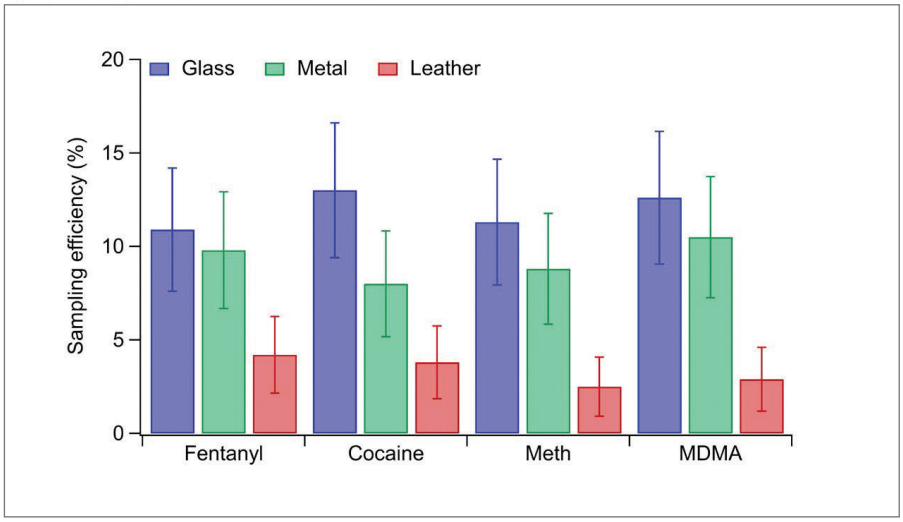
Cocaine	0.47	304.2	182.0
Dexmedetomidine	1.22	201.1	95.1
Fentanyl	0.39	337.2	188.1
Heroin	2.30	370.2	165.1
Ketamine	3.11	238.1	125.1
MDMA	0.73	194.1	163.0
Methamphetamine	1.45	150.1	119.1
Norfentanyl	0.41	233.2	84.1
Oxycodone	0.84	316.2	298.1
Xylazine	0.63	221.1	164.1

Illicit Drug Detection and Identification Using the Continuity™ Field Portable Mass Spectrometer

The BaySpec Continuity™ Portable Mass Spectrometer is equipped with a Swab-based APCI source for on-site field detection of narcotics

By Krisztian Torma, Nathan Grimes



Illicit drug trafficking and abuse present significant challenges for law enforcement and public safety agencies. Traditional drug detection methods often require laboratory analysis, which can be time-consuming and impractical for field use. The need for rapid, on-site identification of illicit substances has led to the development of portable mass spectrometry systems, offering real-time, high-sensitivity detection.

The Continuity™ Field Portable Mass Spectrometer, equipped with a Swab-APCI ionization source, provides a powerful solution for detecting trace amounts of illicit drugs directly from surfaces. Designed for use in security checkpoints, border crossings, and law enforcement operations, the system enables rapid sampling and analysis. Using a simple swabbing process, drug residues from vehicle interiors, clothing, and personal belongings are vaporized and analyzed in seconds. The instrument performs tandem mass spectrometry (MS^2), enhancing specificity by confirming the molecular structure of detected substances.

To assess the system's sensitivity and reliability, calibration curves were generated for ten drug standards, including fentanyl, cocaine, methamphetamine, and MDMA. Recovery studies on glass, metal, and synthetic leather surfaces demonstrated consistent detection capabilities, with TSA-approved cotton swabs ensuring uniform sampling conditions. The limit of detection (LOD) was defined as five times the baseline noise in MS^2 mode, ensuring precise identification of trace-level drug residues.

Results showed that the Continuity™ system effectively detects sub-nanogram quantities of drugs. The LODs for fentanyl, cocaine, and MDMA were determined to be 0.39 ng, 0.47 ng, and 0.73 ng, respectively, confirming the system's ability to identify even minute traces of illicit substances. Recovery studies indicated average recovery rates of 11 percent from glass, 8 percent from metal, and 4 percent from synthetic leather. Given the established LODs, the amount of residue required for detection on a sampled surface is in the sub-microgram range, typically invisible to the naked eye.

With its rapid analysis time, ease of use, and high sensitivity, the Continuity™ portable mass spectrometer offers law enforcement and security personnel an advanced tool for combating drug trafficking. As illicit drug threats continue to evolve, integrating real-time mass spectrometry into field operations enhances detection capabilities and strengthens efforts to prevent the distribution and abuse of dangerous substances.

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