The Application Book 2024

Recent application notes across a range of exciting topics

the Analytical Scientist

Real-Time Measurement of EPA Regulated HON Compounds and Environmental Pollutants Using SIFT-MS

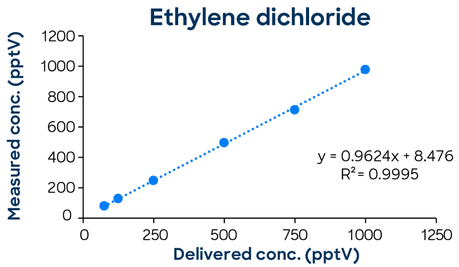
One-minute methods for measuring hazardous air pollutants demonstrate low- to mid-parts per trillion by volume (pptV) sensitivity

Method detection limits (MDLs) have been determined for the newly regulated HON (Hazardous Organic NESHAP (National Emission Standards for Hazardous Air Pollutants)) compounds, which demonstrate selected ion flow tube mass spectrometry (SIFT-MS) as an effective solution for measuring these toxic volatile organic compounds (VOCs) and other environmental pollutants. Hazardous air pollutants can be measured down to the low- to mid-parts per trillion by volume (pptV) range using the one-minute methods described in this application note. SIFT-MS is used by both governmental agencies and industrial manufacturers worldwide for monitoring environmental pollutants.

Compound	MDL (pptV)	HON Action Level (pptV)
Vinyl chloride	460	1170
1,3-Butadiene	60	1360
Benzene	50	2820
Ethylene oxide	105†	110
Ethylene dichloride	260	990
Chloroprene	145	220‡

†EtO MDL over 30 minutes in presence of 2.5 ppbV acetaldehyde (see Discussion).

‡There is a second, lower chloroprene action level (83 pptV) for HON facilities collocated with neoprene production sources (see Discussion).



Low concentration calibrations using simple one-minute methods exhibit excellent linearity down to low pptV concentrations.

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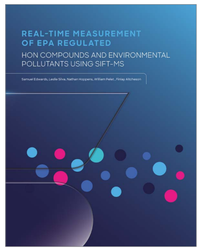

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Learn about Next-Gen Product Solutions

Learn about SyftEnviro mobile monitoring software

See examples of SIFT-MS environmental monitoring in Korea

Comparison of Thyme Varieties from Different Geographical Origins

LECO's new Pegasus BTX promises ultimate sensitivity and revamped ion path integrity

The aroma profiles of herbs, spices, and other natural products play a crucial role in the flavor, food, and fragrance industries. Understanding their chemical compositions is key to determining how these compounds influence aroma. By identifying the chemical makeup of thyme and its origins, businesses can respond more swiftly to consumer and market demands, resulting in more efficient problem-solving and better outcomes.

In this study, the Pegasus BTX GC-TOFMS system and ChromaTOF Sync were employed to analyze and compare dried thyme samples. Comprehensive, non-targeted data were collected across a full mass range with enhanced sensitivity, facilitating efficient deconvolution and thorough detection of analytes in these complex samples.

ChromaTOF Sync enabled the statistical alignment and differentiation of analytes across the sample set, streamlining the comparison and interpretation process. Numerous unique analytes with intriguing aroma profiles were identified in each thyme sample, and the alignment process allowed for the rapid and efficient identification of distinguishing compounds between the four thyme origins.

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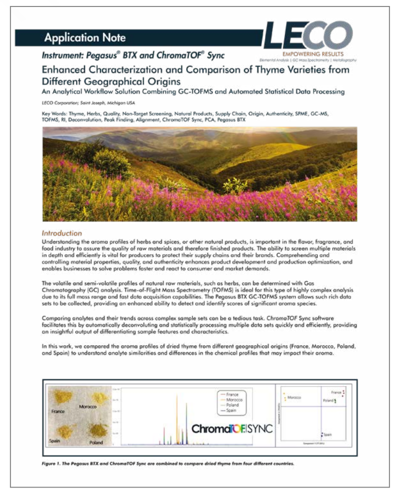

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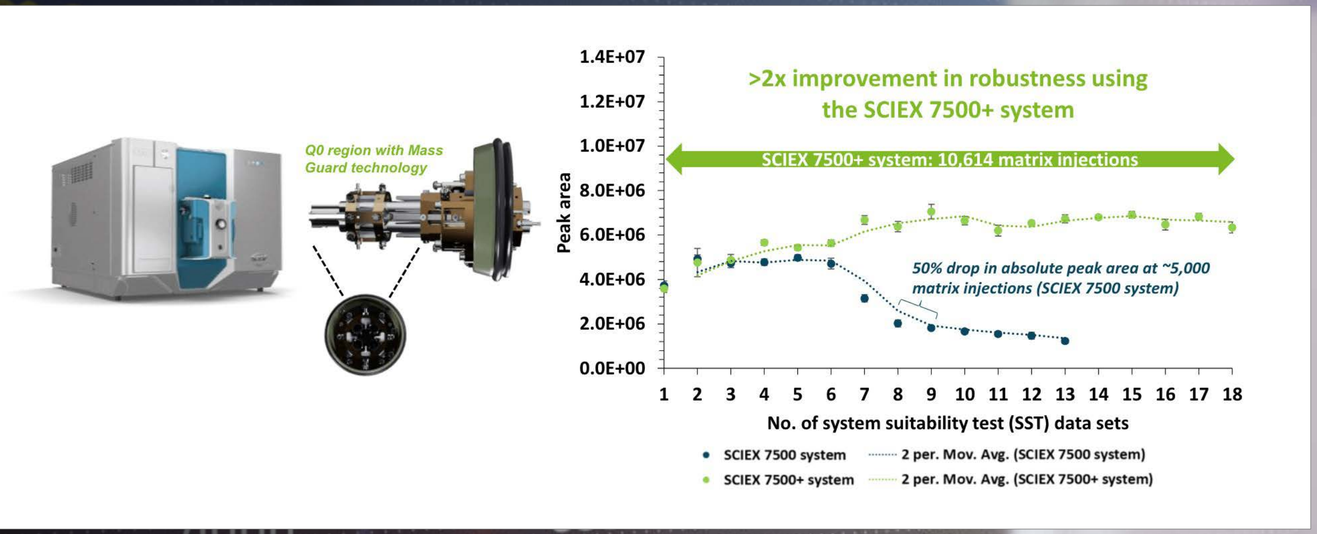
Redefine Bioanalysis with Enhanced Robustness on the SCIEX 7500+ System

A powerful tool for bioanalysis in complex matrices that integrates unparalleled sensitivity and the highest levels of data stability

By Ebru Selen, Rahul Baghla, Ian Moore, Eshani Galermo, Zoe Zhang and Elliott Jones

Here are the key benefits of long-term analysis using the SCIEX 7500+ system:

- **Enhanced robustness with Mass Guard technology:** Perform long-term bioanalysis seamlessly and reduce the risk of instrument downtime due to contaminating ions
- **Exceptional instrument stability:** The SCIEX 7500+ system achieved >2x improvement in robustness, as demonstrated by >10,000 injections of rat plasma matrix
- **User accessibility to the DJet+ assembly:** Easily perform front-end cleaning to minimize unscheduled downtime and maintain instrument performance
- **Built-in contamination check procedures in SCIEX OS software:** Enables easy monitoring of instrument performance for quick troubleshooting



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Read about the SCIEX 7500+ system

SCIEX presents the SCIEX 7500+ system, unveiled at ASMS 2024

Improved Proteomics Performance for Low Sample Loadings

Unlocking high sensitivity and speed for low-abundance protein biomarker detection

By Ihor Batruch and Patrick Pribil

Protein biomarker research aims to identify quantifiable, biologically relevant markers for disease study and clinical treatment. These protein biomarkers often exist at trace levels in biological matrices or tissues, necessitating complex methodologies and instrumentation for their detection and quantitation.

Advances in mass spectrometry technologies that can improve the characterization of low-level biomarkers are highly important; and data-independent acquisition (DIA) workflows are commonly utilized due to their relative simplicity and the depth of information they yield. Unlike discrete-window DIA methods such as Zeno SWATH DIA, ZT Scan DIA uses a continuously scanning quadrupole to isolate precursor ions for fast, sensitive, time-of-flight (TOF) detection. The added specificity in the quadrupole dimension significantly improves the identification and quantitation of peptides and proteins compared to Zeno SWATH DIA.

This technical note highlights the unique benefits of ZT Scan DIA at low on-column loadings using microflow and nanoflow liquid chromatography (LC) – approaching single-cell levels, with quantifiable protein group and precursor detections increased by as much as 50 percent. ZT Scan DIA improves quantifiable identifications at higher throughput LC regimes. This feature is also highlighted in this work with low sample loadings – ZT Scan DIA delivers equivalent performance to Zeno SWATH DIA with significantly shorter microflow or nanoflow LC gradients, enabling users to obtain biologically relevant results faster.

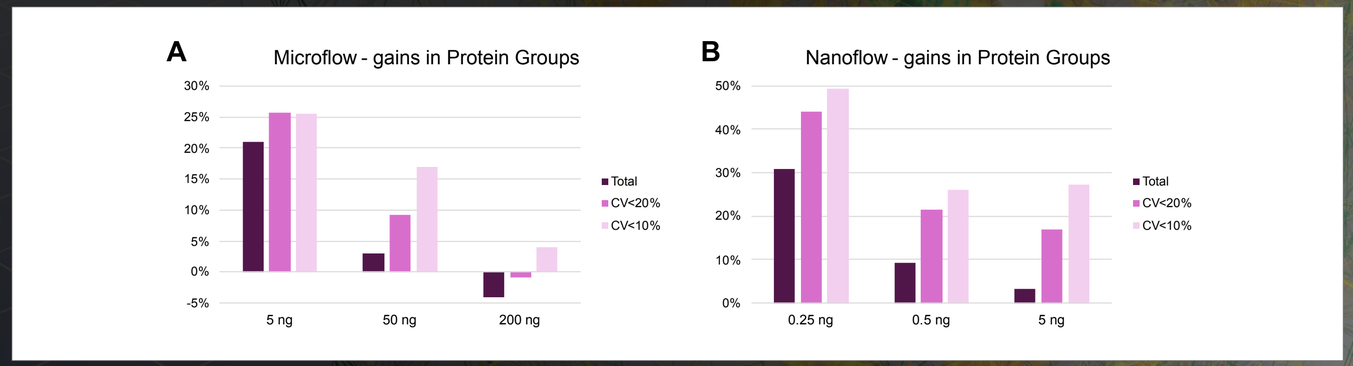

Figure. Gains in the identification and quantitation of K562 protein groups at low sample loadings with ZT Scan DIA. The gains in total protein groups, as well as those quantifiable with CVs <20% or CVs <10%, are shown relative to Zeno SWATH DIA for different on-column loadings of K562 tryptic digest using 15-minute microflow gradients (A) or 30-minute nanoflow gradients (B). Data was acquired in triplicate and processed using DIA-NN software v1.8.1.

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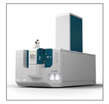
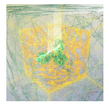
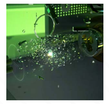
Explore the ZenoTOF 7600+ system



ZT Scan DIA for quantitative proteomics



Delve into the world of Extraordinary Science



High-Resolution Accurate-Mass Library for Forensic Toxicology Screening of Suspect & Unknown Substances

Perform forensic toxicology screening for drugs of abuse, psychotropic drugs, pharmaceuticals, pesticides, and natural toxins using the HR accurate-mass database

By Stephane Moreau

Mass spectrometry (MS) has become a cornerstone technique in toxicology screening, enabling the identification and quantification of a wide range of substances, including drugs, metabolites, pesticides, and environmental toxins. The accuracy of the results obtained from mass spectrometry heavily relies on the quality of the database used for analysis. With high resolution MS, an accurate-mass spectrometry database is essential for several reasons.

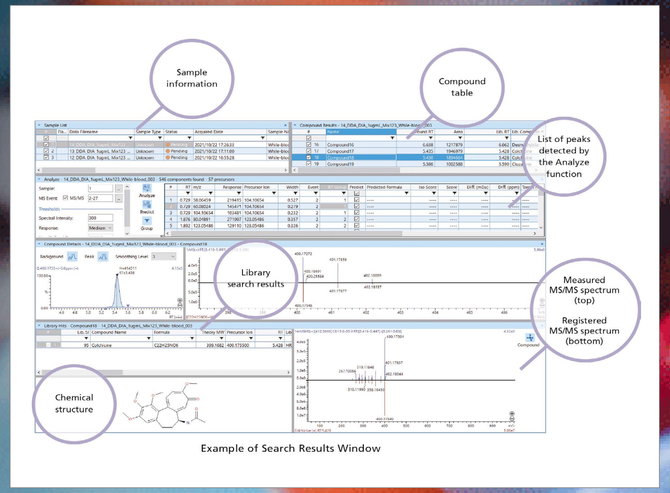
Firstly, the primary function of a mass spectrometry database is to provide reference spectra for comparison. Each compound has a unique mass-to-charge ratio (m/z) and fragmentation pattern, which can be matched against those stored in the database. An accurate database ensures that the identification of compounds is precise, reducing the likelihood of false positives or negatives. In toxicology, where misidentification can have serious implications for patient safety and public health, the need for accuracy is paramount.

Secondly, toxicology often involves analysing complex biological matrices such as blood, urine, and tissue samples. These matrices can contain a multitude of substances, both endogenous and exogenous. An accurate and comprehensive database allows for the effective deconvolution of these complex mixtures, enabling toxicologists to identify not only the primary compounds of interest but also potential metabolites and by-products that may have toxic effects.

Moreover, the evolving nature of toxicology demands that databases are regularly updated to include new compounds, emerging drugs, and environmental toxins. An up-to-date database enhances the capability of toxicologists to respond to new challenges and emerging threats.

Finally, regulatory compliance is another critical factor. Many industries, including pharmaceuticals and environmental monitoring, are subject to strict regulations that require accurate toxicological assessments. Utilizing a reliable mass spectrometry database helps ensure compliance with these regulations, safeguarding public health and maintaining industry standards.

In conclusion, the necessity of using an accurate-mass spectrometry database in toxicology screening cannot be overstated. It is crucial for precise identification, effective analysis of complex samples, adaptation to emerging threats, and adherence to regulatory requirements. Investing in high-quality curated databases is essential for the advancement of toxicology and the protection of public health.



Example of Search Results Window

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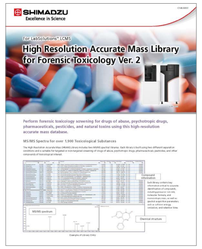

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Product page

LabSolutions Insight Explore

Qualitative analysis of drug metabolites using the LCMS-9050 Q-TOF

Advances in Carbon Quantum Dots: Synthesis, Applications, and Spectral Analysis with Spectroscopy

Discover the future of nanotechnology with carbon quantum dots (CQDs)

As the field of nanotechnology continues to evolve, carbon quantum dots (CQDs) are emerging as a groundbreaking solution with immense potential in biomedical, environmental, and energy applications. Avantes' application note dives deep into the innovative world of CQDs and their growing role in cutting-edge research and industry.

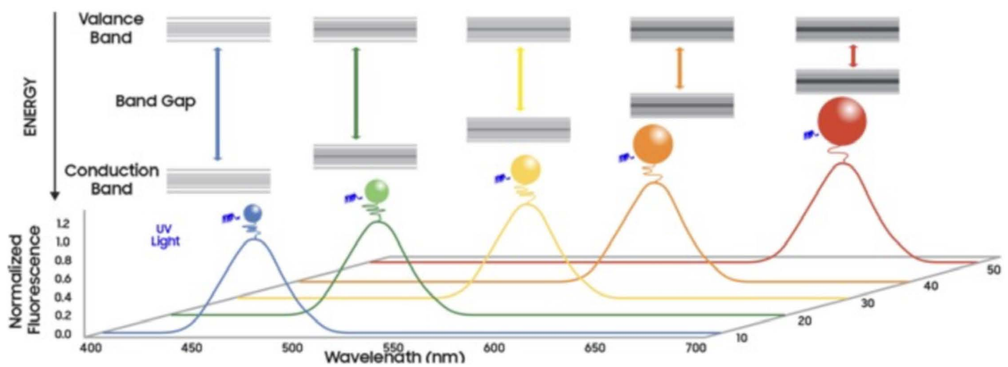

FIGURE 1: *Schematic Illustration of the relationship between quantum dot, size, bandgap and emission spectra.*

Carbon quantum dots and their unique properties
Carbon quantum dots have captivated researchers due to their tunable fluorescence, biocompatibility, and eco-friendly synthesis methods. Unlike traditional semiconductor quantum dots, CQDs present a safer, non-toxic alternative, making them ideal for applications in fields like bioimaging, drug delivery, and sustainable energy solutions. Their small size and highly reactive surface chemistry allow for extensive customization, enabling precise control over their optical properties.

The role of spectroscopy
Understanding the optical and chemical properties of CQDs is essential for unlocking their full potential. Spectroscopic analysis plays a crucial role in this process, providing detailed insights into the emission profiles, structural composition, and behavior of these materials. Using advanced Avantes spectrometers, researchers and manufacturers can analyze CQDs with the precision and accuracy needed for groundbreaking discoveries and large-scale commercial scalability.

Applications in energy, healthcare, and beyond
Carbon quantum dots are paving the way for innovative solutions across multiple industries, from next-generation LEDs and solar cells to medical imaging and drug delivery systems. Our application note highlights these exciting developments and showcases how researchers are leveraging CQDs in cutting-edge technologies.

Explore the full story
Want to learn more about this subject? Download the full application note to explore their synthesis, applications, and the critical role of Avantes spectrometers in driving this research forward.

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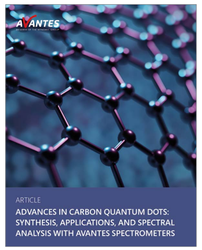

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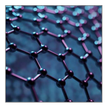


Cases

Markets

Large-Area Wafer Inspection with Raman Imaging Microscopy

Compound semiconductor properties revealed with profilometry-guided Raman analysis

By Thomas Meyer

Raman imaging can determine the chemical composition of a sample, visualize component distribution, and characterize properties such as crystallinity, strain, stress or doping. This is particularly valuable for compound semiconductors, which often consist of multiple elements and complex structures.

In this example, the complete surface of a 150 mm (6 inch) silicon carbide (SiC) wafer was imaged with Raman microscopy using a 532 nm laser for excitation. The instrument employed was a WITec alpha300 Semiconductor Edition Raman system equipped with active vibration damping, WITec Suite data acquisition and post-processing software with TrueComponent Analysis™, the TrueSurface™ profilometry module for closed-loop focus stabilization, and a UHTS 600 ultrahigh-throughput spectrometer.

TrueSurface recorded the wafer's topography simultaneously with the Raman data to compensate for height variations and obtain a sharp large-area image, which also facilitated the generation of a topographic map of the sample.

The analysis showed that the doping concentration was not homogeneous over the full area. The highly sensitive spectrometer was able to detect peak shifts well below 0.01 cm^{-1} and could thus reveal stress fields within the wafer.

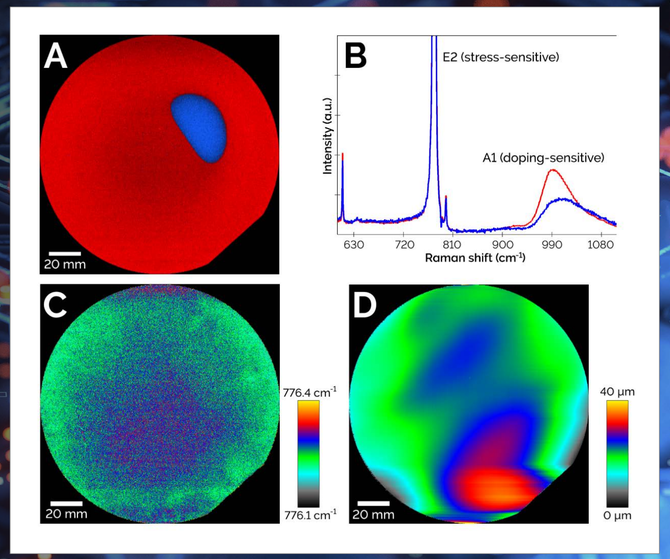
Results

a) Confocal Raman image of a 150 mm SiC wafer. TrueComponent Analysis identified two spectra, which mainly differed in the doping-sensitive A1 peak (ca. 990 cm^{-1}). The image reveals an oval region (blue) with a different doping concentration than the bulk wafer area (red).
b) Raman spectra of the two components identified.
c) Confocal Raman image of a 150 mm SiC wafer, color coded for the position of the stress-sensitive E2 peak (776 cm^{-1}). The image reveals a small, presumably stress-induced peak shift from the wafer's center toward its edge.
d) Topography of a 150 mm SiC wafer with height variations of up to 40 µm.

The sample was provided courtesy of the Fraunhofer Institute for Integrated Systems and Device Technology IISB, Erlangen, Germany.

Conclusion

This study provides clear experimental evidence of the capabilities and advantages of Raman imaging microscopy combined with optical profilometry for the large-area analysis of compound semiconductor wafers. The distributions of doping concentration, material stress, and topographic variation were characterized and visualized across the complete surface of a 150 mm SiC wafer with exceptional resolution.



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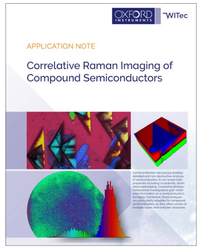

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