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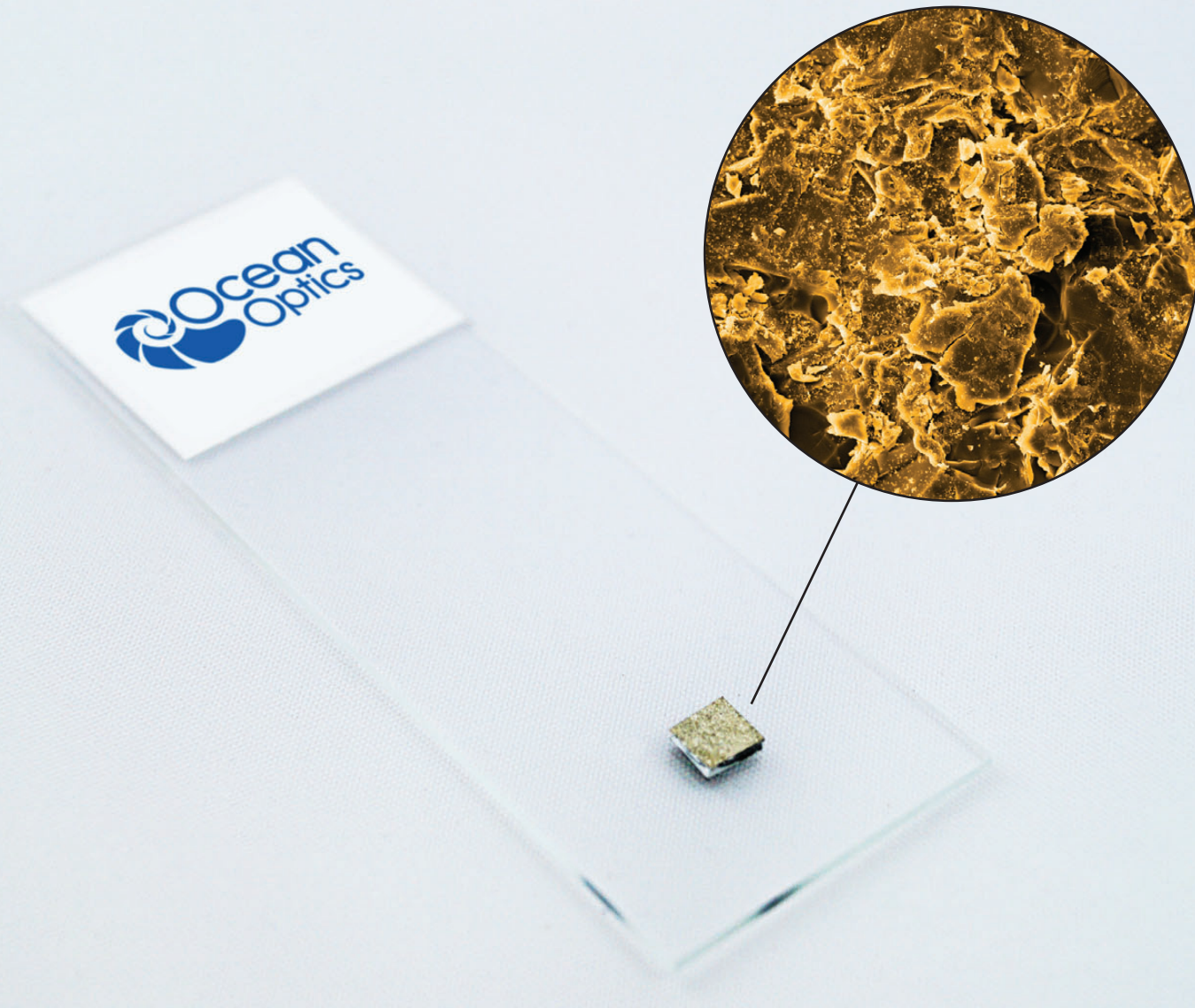


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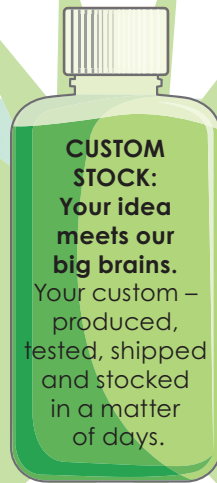
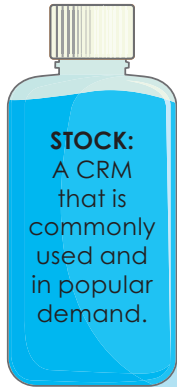
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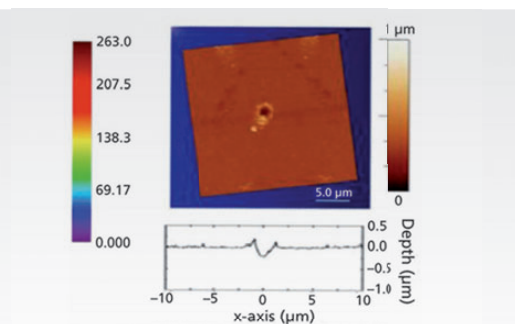
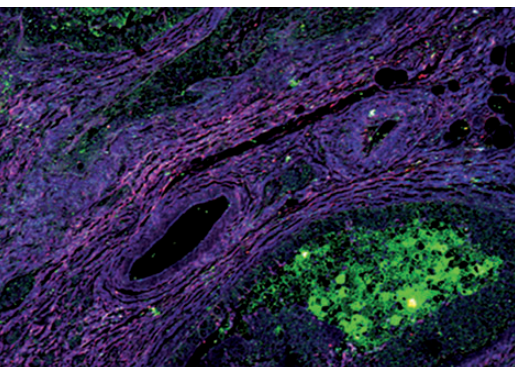


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# Annual Industry Trends & Directory Issue

- 22** SPECTROSCOPIC INSTRUMENTATION: SPECTROMETER SYSTEMS
- 41** OPTICS, ELECTRO-OPTICS, OPTRONICS, FIBER OPTICS, AND RELATED COMPONENTS
- 50** SAMPLING/SAMPLE HANDLING
- 59** SPECTROSCOPY SOFTWARE/COMPUTER HARDWARE/AUTOMATION PRODUCTS
- 62** SPECTROSCOPY SERVICES
- 63** GENERAL SCIENTIFIC EQUIPMENT AND ACCESSORIES
- 70** PROCESS ANALYTICAL INSTRUMENTATION
- 77** BIOANALYSIS INSTRUMENTS

## Also:

- 8** Spectroscopy in Real-World Applications: Current Trends in XRF, LIBS, NIR, QCLs, FT-IR, ICP-MS, and Raman
- 18** PRODUCT INDEX
- 80** MANUFACTURER DIRECTORY

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# Spectroscopy in Real-World Applications: Current Trends in XRF, LIBS, NIR, QCLs, FT-IR, ICP-MS, and Raman

During the past year, *Spectroscopy* examined trends in spectroscopic methods and applications, including advances in X-ray fluorescence (XRF) methods, laser-induced breakdown spectroscopy (LIBS), near-infrared (NIR) spectroscopy, quantum cascade lasers (QCLs), Fourier transform infrared (FT-IR), inductively coupled plasma–mass spectrometry (ICP-MS), and Raman spectroscopy. Discussions of applications in biomedical research as well as the analysis of nanoparticles, pharmaceuticals, environmental samples, and proteins, and more are also presented.

**O**ur interviews with spectroscopy experts in specific application areas, such as biomedical research, the analysis of nanoparticles, pharmaceuticals, environmental samples, and proteins, have provided the *Spectroscopy* audience with insights into the latest trends and developments in those fields. Here, we have excerpted several recent interviews that were published in our print issues and *The Wavelength* newsletter.

## X-RAY FLUORESCENCE SPECTROMETRY

### TOTAL REFLECTION X-RAY FLUORESCENCE SPECTROMETRY FOR METALS AND NANOPARTICLE ANALYSIS

*Spectroscopy* spoke to Ursula Fittschen, an assistant professor at Washington State University, about her work on elemental microscopy and micro analysis. She has been using total reflection X-ray fluorescence (TXRF) to analyze stainless steel metal release, and also airborne silver nanoparticles (NPs) from fabrics. Here, she describes the advantages and challenges of this technique.

*You have used TXRF to perform quantitative analysis of metal release from six different stainless steels in simulated food contact (1). Can you please briefly describe the experimental setup for this study?*

**Fittschen:** In TXRF in contrast to “conventional” XRF the sample is irradiated under a very shallow angle below the critical angle for the given energy and the material of the sample support (which needs to be very flat and smooth). This shallow angle results in a very low penetration depth of the primary beam of <5 nm and therefore very low background. The main advantage of TXRF is its microanalytical capabilities. Less than 1 mg of sample may be used with detection limits in the parts-per-billion range for most elements.

*What are the advantages of using TXRF for stainless steel metal release analysis over techniques such as atomic absorption spectroscopy, graphite furnace atomic absorption spectroscopy (GFAAS), and inductively coupled plasma–mass spectrometry (ICP-MS) and optical emission spectroscopy (ICP-OES)?*

**Fittschen:** The main advantages of TXRF compared to the techniques mentioned above are its microanalytical capabilities along with capabilities to analyze slurries, without the need to digest the sample. (We have used that approach to determine elements with respect to recycling of smelter slag [2].)

Additionally, the small laboratory footprint of the system and low maintenance cost (no consumable besides electrical power) are advantages over most of the techniques mentioned above, which require ultrapure argon. However, here we have used TXRF mainly because of the ability to analyze all relevant elements simultaneously (in general not possible with flame atomic absorption spectroscopy or GFAAS) without the need to optimize plasma conditions for the matrix or individual line (ICP-OES) and without the risk of contamination of the instrumentation, which is a major concern for ICP-MS instrumentation.

*In a recent paper, you used TXRF to analyze airborne silver nanoparticles (NPs) from fabrics (3). What were some of the challenges in developing this method? (For example, interferences or sampling challenges.)*

**Fittschen:** We used a low-pressure impactor to achieve the necessary cutoffs for the NPs and had to modify the impactation plates in a way that allowed us to collect the aerosol directly on TXRF sample carriers. Another challenge was the interference of the Ag L $\alpha$  line with the Ar K $\alpha$  line, which we solved by setting the instrument under a nitrogen atmosphere.





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**What methods were used in the study of silver nanoparticles released from fabrics to confirm your TXRF results, and why?**

**Fittschen:** We used an “on the carrier” digestion and subsequent ICP-MS analysis for confirmation of the presence of Ag in the aerosols. The main problem for this procedure was in the uncertainty of the digestion procedure (the number of digested aerosol deposits and the efficiency of the digestion).

**What are your next steps?**

**Fittschen:** Besides the application of TXRF, we recently published two papers on fundamental aspects of TXRF analysis (4,5), and a paper on a synchrotron setup allowing for TXRF–X-ray near edge structure (XANES) analysis at BESSY II (6). We are about to publish results on studies on the micro-ionome in *Arabidopsis thaliana* making use of TXRF microanalytical capabilities.

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## LIBS

### LIBS AT THE SUBMICROMETER SCALE

*Spectroscopy* spoke to Vassilia Zorba of Lawrence Berkeley National Laboratory in Berkeley, California, about what her studies have revealed about the mechanisms of plasma emission at small scales and what she has found when applying femtosecond laser-

induced breakdown spectroscopy (LIBS) to the study of advanced battery materials.

**You have been exploring femtosecond LIBS at the micrometer and submicrometer scale. What drove you to apply LIBS to analysis at this scale?**

**Zorba:** In any elemental analysis or elemental imaging application, the spatial resolution has to be commensurate with the size of the smallest feature that we want to chemically resolve. For many types of advanced material applications, such as next-generation-energy related materials (generation, conversion, storage), particle analysis, thin films, and interfaces, the resolution requirements usually range from the nanometer to submicrometer scale. Spatial resolution in LIBS is defined by the size of the ablation crater and is typically several tens to hundreds of micrometers in diameter (macroscale). Our focus is on pushing LIBS to smaller length scales and its use in high-resolution elemental imaging in some of these emerging applications.

**What makes measurements at these small length scales a challenge? What are the advantages of using femtosecond LIBS at that scale?**

**Zorba:** Laser-induced plasma emission at the submicrometer scale is a “black box.” There is very little that we know about plasma properties and emission mechanisms and how they compare to the macroscale. Better resolution in LIBS means that we are ablating less mass and therefore detection of the emission may be quite challenging. The best we can currently do in terms of spatial resolution with femtosecond LIBS is a little less than 500 nm, corresponding to absolute limits of detection of the hundreds of attograms (1).

Femtosecond lasers are ideal for high-resolution LIBS. This has to do with their fundamentally different laser–material interaction compared to nanosecond lasers. Nonlinear absorption enables spatial and axial confinement of the femtosecond laser beam, and suppressed thermal effects reduce signs of sample melting, resolidification, and thermal load on the sample. All of these parameters help us achieve precise sampling with well-defined craters, which under certain conditions may even be below the diffraction limit.

**In a recent study (2), you used femtosecond LIBS to analyze copper at the micrometer and submicrometer scale, and studied the LIBS spectral emission characteris-**

**tics and the plasma properties. What did you find about how the spectral emission characteristics and plasma properties of femtosecond LIBS at the micrometer and submicrometer scale differ from those at the macroscale?**

**Zorba:** This study showed that the electron number density and excitation temperature are really not that different from those reported in macroscale femtosecond LIBS, despite the fact that the ablated mass is orders of magnitude smaller (see Figure 1 on-line for an example of results obtained in the study, [www.spectroscopyonline.com/libs-submicrometer-scale](http://www.spectroscopyonline.com/libs-submicrometer-scale)). Intuitively we expect that the less mass we have, the smaller the LIBS signal intensity will be, which is true. However, the emission efficiency—the ratio of the emission intensity over the ablated material volume—is reduced as we scale down in mass. In other words, it's not just that we have less mass, but that a smaller percentage of species in that mass lead to detectable LIBS emission.

**What does this information tell us about how to improve femtosecond LIBS or how to better harness its capabilities?**

**Zorba:** These results really give us a first insight into the mechanisms of plasma emission at small scales. It is inevitable that after a certain point when the ablated mass is very limited (less than attogram scale), we will no longer detect LIBS spectral emission in the optical far-field. At this scale, secondary excitation mechanisms start to become much more significant so that we can re-excite or reheat the existing plasma. To maintain the spatial resolution provided by the femtosecond laser ablation, it is important to look for approaches in which the secondary source only interacts with the plasma and not the sample. One of the more straightforward approaches for this is orthogonal double-pulse LIBS, where the ablation and re-excitation pulses are perpendicular to one another.

**Large concentrations of nanoparticles are known to be present in femtosecond-laser-induced plasmas at the macroscale. What is the influence of nanoparticles in the plasma in femtosecond LIBS at the micrometer and submicrometer scale?**

**Zorba:** In previous work on ultraviolet femtosecond–nanosecond double-pulse LIBS at the micrometer scale, we found that emission intensity enhancement of two orders of magnitude is possible for Si at these small length scales (3), which is quite significant, especially



considering how little ablated mass there is to begin with. In that work we demonstrated evidence for the presence of nonradiative species or particles in small-scale plasmas that remain long after LIBS emission has ended. The differences we observed in emission efficiency (2) may be attributed to an increasing concentration of nonemitting nanoparticles versus emitting species as we scale down in laser energy and crater sizes.

**You have used femtosecond LIBS to study the solid electrolyte interphase (SEI) in rechargeable lithium-ion batteries (4). What is the SEI and why is understanding it important for improving the performance of these batteries?**

**Zorba:** The SEI is a thin interfacial layer with a thickness of a few tens of nanometers that forms spontaneously on Li-ion battery electrodes upon the early stages of charging in liquid electrolytes. This interfacial layer affects the entire cell electrochemical behavior, cell lifetime, and safety performance. The SEI is also thermodynamically unstable with nonuniform composition and morphology. Because of the SEI's direct impact on battery performance, controlling the SEI's exact composition and understanding its formation mechanism is considered one of the greatest challenges in Li-ion battery fundamental research.

**What advantages does LIBS have for studying the SEI, compared to other techniques?**

**Zorba:** Because of the thinness of the SEI layer, there is a need for techniques that can provide information on its chemical composition with very high depth resolution (<10 nm). Figure 2 (available on-line, [www.spectroscopyonline.com/libs-submicrometer-scale](http://www.spectroscopyonline.com/libs-submicrometer-scale)) shows results from the femtosecond LIBS analysis of a highly oriented pyrolytic graphite layer at a depth resolution of 7 nm. At the same time, characterization can be difficult because of the instability of the layer; handling the material in air or transferring it to vacuum may affect the chemical composition or mechanical stability of the layer, or both. The advantages of femtosecond LIBS for the characterization of SEI layers are that as an all-optical technique, femtosecond LIBS allows analysis in their inherent environment (a He or Ar atmosphere is common ex situ), it can provide information as a function of depth, and it is a technique that is inherently very sensitive

to Li. This is a fairly unique combination of characteristics that is extremely hard to find in most spectroscopic techniques.

**You have also used femtosecond LIBS to carry out three-dimensional elemental imaging of  $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$  (LLZO)—an alternative solid-state material for Li-ion batteries (5). Why is it necessary to study these materials at this scale? What can femtosecond LIBS reveal about these materials that other techniques cannot?**

**Zorba:** LLZO is a solid-state electrolyte,

which is a safer material for large-format Li-ion battery applications such as electric vehicles. Partial Al-substitution in LLZO, which is used to stabilize the cubic structure, introduces new impurity phases, chemical composition changes, and elemental distribution gradients at surfaces, at grain boundaries, and in the bulk of the material. Because of their low concentrations and distribution patterns, these impurities, changes, and gradients are often difficult or impossible to detect by conventional characterization techniques, but they still greatly affect the electrochemical

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properties of LLZO.

Some of the more common techniques used for the analysis of solid-state electrolytes such as LLZO are inductively coupled plasma–optical emission spectroscopy (ICP-OES) and ICP-mass spectrometry (ICP-MS), which do not provide spatially resolved information, and energy-dispersive spectroscopy (EDS), which is limited to surface composition and has reduced sensitivity to Li. We found that femtosecond LIBS is a very powerful technique that provides high sensitivity two dimensionally (2D) layer-by-layer, in 2D cross-sectional analysis, and for three-dimensional (3D) imaging, all of which allow us to visualize the distribution of major and minor elements of interest in LLZO matrices. This information, combined with complementary spectroscopies and electrochemical characterization, is important for improving the fabrication process of solid-state electrolytes.

**Why was 3D mapping important in this study? And are there any significant challenges to converting the data into 3D maps?**

**Zorba:** Visualization of the distribution of the elements in the LLZO matrix was important to extract the atomic ratios of major and minor elements below the material surface, and to find correlations with their electrochemical behavior (Figure 3, available on-line at [www.spectroscopyonline.com/libsubmicrometer-scale](http://www.spectroscopyonline.com/libsubmicrometer-scale)). The main challenge in data visualization is that as the resolution (spatial or axial) increases, the amount of spectra and data become increasingly hard to process and reconstruct. In addition, transitioning from layer-by-layer maps to the 3D space requires use of protocols for computational reconstruction. Advancement of visualization techniques and strategies for handling big data will be important in the next few years for expanding LIBS into a true 3D chemical imaging technique.

**The LLZO solid electrolyte material was prepared for LIBS analysis as pellets covered by fresh LLZO powder and by LLZO powder that was annealed at a high temperature for several hours. What did you learn about how your sample preparation affected your results?**

**Zorba:** We found that small variations in the sample preparation method affected the distribution of low-concentration Al and its segregation at specific locations in the material matrix. This variation in subsurface

composition, along with microstructure and electrochemical parameters, resulted in a significant decrease in the sample conductivity and increase of the interfacial resistance (6). This was a very good example of how small variations in subsurface composition can really affect performance, and how important elemental imaging can be used to control fabrication processes of next-generation energy materials.

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## NIR ANALYSIS

### FROM PHARMACEUTICAL TO AGRICULTURAL APPLICATIONS: WHAT'S NEW IN NIR?

Benoît Igne, a principal scientist at GlaxoSmithKline in King of Prussia, Pennsylvania, spoke to *Spectroscopy* about his work using NIR and areas where he thinks the technique has growth potential, specifically process analytical technology and agriculture.

**Your work experience has explored how NIR spectroscopy can be used to better control pharmaceutical manufacturing. How did you get involved in that area? What was the most interesting thing you discovered about NIR for pharmaceutical manufacturing?**

**Igne:** I have always been interested in measuring quality. During my master's degree studies in Toulouse, France, I worked with food companies to predict quality parameters using IR and NIR. As I carried on my graduate education at Iowa State University, I applied NIR to the measurement of grains and feed. I chose this area of study because I have never been attracted to wet

chemistry and the related sample preparation and slow outputs. I have found NIR to be a very satisfying measurement technique where the analysis is made rapidly, without sample preparation, and can provide comparable results to its wet chemistry equivalent. I am also very interested in how chemometrics can be used to extract the relevant information from the spectra, similar to how a chromatography column separates out the components of interest. When I joined Duquesne University, I started using NIR and chemometrics for pharmaceutical issues. I found the possibility of building an entire dataset using synthetic powders very convenient. In contrast to agriculture and other fields impacted by growth cycles, in the pharmaceutical industry it is possible to develop methods a lot more efficiently.

**In the preface to the second edition of your book (1), you comment that regulatory documents issued by the FDA, EMA, and ICH, starting in 2002, have “. . . helped position near-infrared spectroscopy as a highly relevant tool for achieving control when built-in quality is preferred over quality by testing.” What is your assessment of the progress that has been made in using NIR and similar methods for process control, since the agencies started issuing those documents in 2002?**

**Igne:** While the documents issued by national and international agencies do provide a framework within which to work, I think the industry is still struggling to comfortably submit files that include process analytical technology (PAT) as a tool for some sort of decision on the process or batch release. One of the common sticking points is related to calibration updates. Like every analytical tool, PAT requires model maintenance. It is, however, the complexity of the requirements around the submitting these updates or adjustments to registered methods with the FDA or another regulatory agency that add complexity to the long-term deployment of these tools. Progress has certainly been made but processes can be further simplified.

**How does NIR research fit into your agricultural background? Are there any agricultural areas you see as potential future applications for NIR?**

**Igne:** In agriculture, you want to be able to make decisions quickly based on reliable



data. NIR has positioned itself as a great tool to be able to provide some of the information farmers are looking for. Combine harvesters can now be equipped with NIR sensors to provide the mapping of fields, using a GPS device, based on product quality. Soils can also be analyzed from the ground or by using remote sensing imaging solutions. These data can, for instance, be used in subsequent years to adapt fertilization plans to local heterogeneities and increase yields. As instrument manufacturers provide smaller and more cost effective sensors, we can expect NIR to be deployed not only in centralized locations but also more widely. Bringing the information directly to those in charge of making the decisions in the field may be the next frontier for NIR in agriculture.

***Do you think NIR will ever see significant adoption beyond process applications, and be used in the laboratory?***

**Igne:** While there are numerous NIR applications in the laboratory (off-line) or at-line, most of the advantages of the technology are certainly found in process monitoring and control. What makes NIR so suitable for processes (relatively low sample absorbance allowing some depth of penetration, rapid acquisition, limited to no sample preparation, and so on) is also what makes it less attractive than other methods for laboratory applications (sensitivity to sample physical properties, overlapping bands). In the laboratory, NIR applications could be replaced by techniques such as transmission Raman; but it is not clear, for the time being, that any other technology can replace the flexibility that NIR provides in process monitoring and control.

***What are the next steps in your work?***

**Igne:** Value from the deployment of PAT techniques can be obtained through a number of avenues: improved process understanding allowing shortened development time, real-time assurance, real-time release testing, and so on. However, NIR, along with other PAT tools, cannot be solely used for making decisions on processes. It is the integration of the outputs from PAT tools with statistical process control and automation that provides the possibility to monitor and control a process. This is the area that I am progressively going toward, and I hope to be able to use NIR and other tools to work on setting up fully integrated control

systems to guarantee product quality and ensure patient safety.

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## QUANTUM CASCADE LASERS

### MINIATURIZED QUANTUM CASCADE LASERS ENABLE FAST MID-IR SPECTROSCOPY

*Spectroscopy* spoke to Ralf Ostendorf of the Fraunhofer Institute for Applied Solid State Physics (IAF), in Freiburg, Germany, about his work on the development of a miniaturized quantum cascade laser (QCL), which when used as a light source, enables mid-infrared (mid-IR) scanning speeds much faster than those of conventional Fourier transform IR (FT-IR).

***In a recent paper (1), you presented information that showed how an external-cavity quantum cascade laser (EC-QCL) equipped with a custom made micro-opto-electro-mechanical systems (MOEMS) scanning grating in Littrow-configuration can be used in wavelength-dependent feedback element in a mid-IR EC-QCL, featuring a large scanning grating plate 5 mm in diameter. How does this technique improve on current techniques?***

**Ostendorf:** Initially, our goal was to miniaturize the laser source. We wanted to build a compact, matchbox-sized laser source and demonstrate the capability of laser-based mid-IR laser spectroscopy in different applications. We started a collaboration with our colleagues from the Fraunhofer Institute for Photonic Microsystems (IPMS) in Dresden, who are experts in developing MOEMS technology. Our idea was to use a small silicon chip with an implemented diffraction grating (so called MOEMS grating) as a wavelength selective element and combine it in an external cavity with a quantum cascade laser chip developed at Fraunhofer IAF. Both chips are pretty small, just a few millimeters, so we saw an enormous potential to miniaturize the laser source. The MOEMS grating is tilted by electrostatic forces and is driven in a resonant way, meaning it is tilting continuously with frequencies of up to

several kHz. At this point we realized that we could also perform very fast spectroscopy even in real-time.

The innovation in this MOEMS EC-QCL, apart from the fact that it is no bigger than a matchbox, is that it is able to tune the wavelength over a broad spectral range of more than 300  $\text{cm}^{-1}$  in the mid-IR within just one millisecond. Using this laser as a light source for mid-IR fingerprint spectroscopy allows for recording of up to 2000 spectra per second (tilting the grating up and down during one period equals two complete wavelength scans) which is far faster than any conventional mid-IR spectroscopy, such as FT-IR spectroscopy. Thus, the MOEMS QCL opens the possibility of identifying and quantifying chemical substances in real-time.

Moreover, due to the spectral brightness of the laser, you can even measure aqueous solutions. Usually, IR light is strongly absorbed by water. If you use common techniques like FT-IR, you are able to measure small water films no thicker than 10  $\mu\text{m}$ . We were able to identify caffeine dissolved in water (25 mg/L) through a 150- $\mu\text{m}$  water film, and there is the potential to go to even thicker water films. This is very attractive for sensing solutions that are operated in a bypass flow cell.

***Why is the tuning speed of an EC-QCL important for applications such as real-time monitoring and in-line process analysis?***

**Ostendorf:** In the end it comes down to the simple equation "time = money." Today, if you want to analyze the chemical composition of a large amount of bulk material, such as pills in pharmaceutical production or nuts in a food processing plant, you need to take random samples, bring them to a lab and perform time-consuming chemical analysis using, for example, FT-IR spectroscopy. The high tuning speed of the MOEMS EC-QCL allows for the development of mid-IR sensing systems that can record 2000 spectra per second. This means in principle you can analyze 2000 nuts or pills per second, allowing for 100% control of your batch during the production process, without the need to take random samples. In this way you can speed up your production while having more control over your process at the same time.

Furthermore, due the high tuning speed of the MOEMS EC-QCL and the fact that the laser is emitting in the mid-IR fingerprint region, where the absorption lines of chemical substances are so characteristic and strong like nowhere else, you can trace a chemical reaction in real-time and see how much of your chemical reactants are already consumed and transformed into the final chemical product. In this way you can optimize chemical reactions on-the-fly, for example, to enhance yield or to speed up production cycles.

**You have applied this technique to monitoring a Knoevenagel condensation reaction, which is a prototypical catalytic chemical reaction. What results have you seen so far?**

**Ostendorf:** The monitoring of the Knoevenagel condensation was performed by colleagues of mine at the Fraunhofer Institute for Chemical Technology (ICT) in Pfinzthal. They still used a “slow” scanning EC-QCL; for example, recording one spectrum from 1050  $\text{cm}^{-1}$  to 1300  $\text{cm}^{-1}$  took about 3–4 seconds. The Knoevenagel condensation was chosen to act as a prototypical catalytic chemical reaction to demonstrate the capabilities of the EC-QCL based spectroscopy for chemical process monitoring. The spectra show that, despite a very low concentration of the involved reactants of 40 mM, very good signal intensity and low noise were achieved, both mostly resulting from the high energy density of the laser source. During the reaction time of about 15 minutes, a clear change in the absorption spectra could be observed. For example, a decreasing absorption band at 1160  $\text{cm}^{-1}$  attributed to the aldehyde group of the educt (4-methoxybenzaldehyde) and a rising absorption band at about 1180  $\text{cm}^{-1}$  attributed to the emerging C=C double bond of the product was monitored. This allowed for the application of chemometric quantification procedures and determination of the product composition during the whole time of the reaction. Based on these data the kinetics of the chemical reaction could be characterized and optimized for yield, conversion efficiency, and the influence of the involved catalyst.

**Can you describe the results you have achieved in applying this technique to the**

**standoff detection of explosives?**

**Ostendorf:** We are still using the “conventional” EC-QCL for the standoff detection of explosives, although we have plans to use our fast scanning MOEMS EC-QCL for this application as well in the near future. The standoff system developed at Fraunhofer IAF is based on a hyperspectral imaging technique. For example, the laser is used to actively illuminate scenery, and while tuning the wavelength of the laser, an IR camera system takes pictures from the diffusely backscattered light for each wavelength. From these data, spectra can be extracted using sophisticated algorithms to identify traces of chemical contaminations in the illuminated scenery, such as the remains of explosives. The group at Fraunhofer IAF developing this technique led by Dr. Frank Fuchs has already successfully demonstrated the reliable detection of small traces of explosives over distances of more than 20 meters. Using the MOEMS EC-QCL approach in the near future will enable real-time capability for this application as well.

**What are your next steps in your research?**

**Ostendorf:** We are currently working on first real-time measurements spectroscopic measurements to demonstrate the capabilities of this technology as well as paving the way for first applications like a handheld sensor for hazardous substances, which is developed within the framework of a joint European Project called “Chequers.” We have already been able to show real-time absorption on a polystyrene sheet and measure a complete absorption band of carbon monoxide over a spectral range of more than 200  $\text{cm}^{-1}$  in real-time.

We are also working further on miniaturizing the laser source and simplifying alignment procedures of the grating and micro-optics to increase the quantity of laser sources we can provide to potential end-users.

On the side of the quantum cascade laser chip, we are trying to widen the spectral tuning range of the laser to be able to address more absorption lines in spectroscopic applications. Regarding the MOEMS grating, we have some ideas with our colleagues at Fraunhofer IPMS to enhance the functionality of the laser source.

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## FT-IR

### FT-IR FOR CANCER DIAGNOSIS

Matthew Baker of the University of Strathclyde in Glasgow, Scotland, spoke to *Spectroscopy* about his work using attenuated total reflection (ATR) and ATR combined with Fourier transform infrared (FT-IR) spectroscopy for the analysis of biological samples. The noninvasive procedure allows for the rapid detection of diseases and provides an opportunity for early administration of a therapeutic strategy, when the treatment is most effective.

**In a recent paper (1), you pointed out that a rapid diagnostic serum test for malignant gliomas, one of the more lethal human cancers, would be beneficial to both patients and clinicians, and would reduce diagnosis times. How does the use of ATR–FT-IR spectroscopy assist in the reduction of diagnosis time?**

**Baker:** In 2013, 38% of brain tumor patients visited their doctor more than five times before diagnosis (2). Following access into the clinic, to the specialist, normally a biopsy is taken—a very invasive procedure—followed by histopathological assessment, which can be subjective. This process can take weeks. ATR–FT-IR could offer a different way for brain tumors to be detected solely from human serum.

**Based on your studies so far, how accurately can an ATR–FT-IR serum test diagnose a specific form of brain cancer? And how does the accuracy of this test compare to the accuracy of tests currently in use?**

**Baker:** From our proof of principle work (1), we have shown that we can differentiate between low-grade gliomas, high-grade gliomas, and non-cancer patient’s serum to sensitivities and specificities as on average of 93.75% and 96.53%, respectively. It is hard for us to assess the accuracy of the test currently in use as of course we are basing our starting test upon agreement between histopathologists, but it has been shown by Bruner and colleagues (3) that disagreements between original and review diag-



noses occurred in 214 out of the 500 cases analyzed, some 42.8%; however, that is not an accuracy comparison between the two techniques.

**What are the biggest challenges involved in applying ATR–FT-IR to cancer diagnosis in serum?**

**Baker:** There are many, unfortunately. ATR–FT-IR is a simple, versatile technique; however, it is not currently clinically used. We have to understand the clinical environment where we are hoping to place the spectrometer to ensure that we are matching what they need and doing it in such a fashion as to cause limited disruption to the current diagnostic process. This is a challenging step because there are always things that you haven't thought about, such as the availability of power or the different times that serum may be collected and processed depending upon staff resources.

**Because of the strong IR activity of water, most biofluids are dried before IR analysis, but there can be inconsistency in the way samples are dried, or in the way they are diluted before drying. In a recent study (4), you studied how to optimize the preparation of biofluid samples for IR analysis. What did you find?**

**Baker:** The study referred to in reference 4 looked at the use of high-throughput IR, which works on transmission, and ATR. The study showed three major points: that a dilution is required before analysis by transmission IR and that threefold dilution was the optimum from reproducibility and repeatability measurements following spectral quality tests; that ATR–FT-IR and transmission IR provide similar peaks and ability in the discrimination of biological spectra; and there will always be a coffee ring effect no matter which format is used, as it is based on sample preparation, and it is best to minimize the effect of that heterogeneity on your model through stringent quality tests.

**What are your next steps in your research?**

**Baker:** We would like to further understand the impact of our sample preparation approach on the spectrum produced and then try to expand to actual clinical tests and other diseases.

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## ICP-MS

### ICP-MS FOR ENVIRONMENTAL AND BIOIMAGING RESEARCH

Uwe Karst, a Professor and Chair of the Analytical Chemistry Department at the University of Münster in Germany, spoke to *Spectroscopy* about the work he and his group are doing using ICP-MS for applications such as analyzing magnetic resonance imaging (MRI) contrast agents in river water, speciation analysis in a study of a disease related to renal failure, and examining the distribution of a labeling compound in mouse tumor cells and macrophages.

**In a recent study (1), you used hydrophilic interaction liquid chromatography (HILIC) combined with ICP–sector field MS to analyze local Münster surface waters for gadolinium-based MRI contrast agents introduced into the environment through a wastewater treatment plant. Your approach optimized the sample introduction into the plasma by means of desolvation. Can you please briefly describe the major features of your method?**

**Karst:** Due to the fact that some of the gadolinium-based contrast agents are anionic, while others are neutral, HILIC separations are the method of choice for their separation rather than ion chromatography. Although peak shapes and loadability of the columns are limited compared to reversed-phase columns, the latter do not show retention of the analytes and can therefore not be applied. In this particular publication, desolvation was used to further improve the limits of detection.

**Was there any particular advantage to using a sector-field MS system in that**

**analysis?**

**Karst:** Despite strong progress in the field of quadrupole-based mass analyzers for ICP-MS, sector-field instruments still offer the best limits of detection, particularly when operated at low resolution. As our approach is limited by the analyte signal itself rather than by the blank—as are many other approaches in the field of speciation analysis—superior instrumental sensitivity is directly transferred into improved limits of detection. Therefore, sector-field ICP-MS still is our preferred instrumentation for speciation analysis at ultratrace concentrations.

**A second paper from your group describes the combination of ICP-MS, laser-ablation (LA)-ICP-MS, and HILIC-ICP-MS in a study of nephrogenic systemic fibrosis (NSF), a rare renal disease that occurs after the administration of gadolinium-based MRI contrast reagents (2). How were each of the three ICP techniques used to their advantage in the study?**

**Karst:** The goal of this work was to provide a simple and efficient strategy for diagnosis of NSF based on the gadolinium concentration in the skin. NSF is characterized by deposits of gadolinium in the skin, presumably together with calcium and phosphorus as gadolinium calcium phosphates. Therefore, the first approach is to simply dissolve a small sample of a patient's skin biopsy in nitric acid and to determine the total gadolinium concentration, ideally in comparison to a skin sample of the same patient, which is not affected by NSF. Only if an increased concentration of gadolinium is found in the sample affected by NSF, do further investigations have to be carried out to unambiguously diagnose the disease. This can best be done by elemental bioimaging using LA-ICP-MS. If high concentrations of gadolinium (mid-ppm range or above) are found and they correlate with the distribution of calcium and phosphorus, the NSF case is confirmed. In this particular study, we also successfully used speciation analysis based on HILIC-ICP-MS to find out if residues of the originally used contrast agents can still be detected.

**Your group has also used LA-ICP-MS to monitor the distribution of lanthanide-complex labeling compounds on mouse tumor cells and macrophages (3). How**

*did the distribution maps obtained using LA-ICP-MS compare with previous MRI data? What were the advantages of the LA-ICP-MS technique for this elemental bioimaging study?*

**Karst:** MRI is one of the most powerful methods for medical imaging. However, the spatial resolution and the degree of chemical information obtained using this technique are limited. LA-ICP-MS is an ideal complementary imaging method to MRI for animal studies, because it provides highly sensitive and spatially resolved, quantitative analysis of the lanthanides, which are contained in the most frequently used MRI contrast agents. LA-ICP-MS allowed us to precisely quantify, based on matrix-matched standards, the concentration of the lanthanide markers in thulium-labeled tumor cells.

*What are the next steps in your research?*

**Karst:** The next steps will be improvements of the spatial resolution in LA-ICP-MS to spot sizes in the 1- $\mu\text{m}$  range, as this will allow us to shift our focus from the tissue level to the cellular level. However, as the decrease of the spot sizes automatically leads to less ablated substance and therefore inferior limits of detection, this strategy will only be promising in those cases where analyte concentrations are not too low. Another important goal is to increase the number of spots analyzed per second, as LA-ICP-MS requires a significant analysis time of up to 50 hours for a single sample. This step requires improved ablation cells and dedicated cells for the ablation of soft (biological) materials.

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## RAMAN

### UV RESONANCE RAMAN SPECTROSCOPY ANALYSIS OF PROTEIN STRUCTURE AND FOLDING

*Spectroscopy* spoke to Sanford A. Asher,

Distinguished Professor of Chemistry at the University of Pittsburgh, about his work using UV resonance Raman spectroscopy to study peptide excited states and conformations and protein folding, with the ultimate goal of helping to advance research into the mechanisms of disease.

*Can you please briefly describe the basics of UV resonance Raman spectroscopy and discuss why it is a useful technique for examining protein and peptide structure?*

**Asher:** Raman is a very powerful technique since it monitors the simultaneous coupling of electromagnetic radiation with the electronic charge localized in particular chromophoric groups of molecules, and the coupling of molecular vibrations with that electronic charge that was forced to oscillate by the driving electromagnetic radiation. This second-order coupling is extraordinarily sensitive to molecular structure and environment, giving rise to a very high information content spectroscopy. In addition, there is high selectivity for vibrations of interest since excitation can be localized within specific chromophoric groups in a sample, such as in particular sidechains in specific proteins. There is also high sensitivity due to the increased resonance Raman cross sections for particular vibrations. This enables trace detection methodologies.

*Your research involves the study of intrinsically disordered proteins (IDPs) that may be involved in disorders such as Parkinson's disease, Alzheimer's disease, and type II diabetes. What is the source of the spectral differences for protein secondary structure (that is, beta sheet versus alpha helix), and how is that information used in your research with these proteins?*

**Asher:** Over the last two decades we demonstrated the unique power of deep UV resonance Raman to determine secondary structure of peptides and proteins. Our method is far more informative than circular dichroism (CD) spectroscopy. We easily differentiate alpha helix from beta sheet and from PPII conformations. The information content allows us to also differentiate  $310$  and  $\pi$  helices and various turns. This enables us to elucidate the

changes in secondary structure of IDPs as they bind their biological targets.

Our most important result is that we can use our spectral data to calculate the secondary Gibbs free energy landscape along, for example, the Ramachandran  $\psi$  angle folding coordinate. This is the first time that this type of reaction coordinate information was available from experiments.

*How can the technique be used in kinetic studies of protein structural changes?*

**Asher:** We can use it to follow dynamics such as protein folding and unfolding. In one experiment we excite a water solution of a protein with a 1.9-mm IR pulse that is absorbed by a water vibrational overtone. This energy is thermalized in picoseconds. We can then excite with a delayed UV pulse to monitor how the secondary structure evolves. These dynamic spectra can be analyzed to construct a movie that shows the secondary structure evolution during unfolding. This uncovers the activation barriers so important in structural evolution.

*What other spectroscopic techniques have you used in your research with IDPs? How does that information complement the results provided by UV resonance Raman spectroscopy?*

**Asher:** We of course utilize all of the standard techniques important in biophysical chemistry. The UV Raman techniques are novel and are motivated and tailored to resolve the existing outstanding questions.

*What are the next steps in your research?*

**Asher:** We are continuing our biological protein folding investigations and are developing addition sophisticated polarized Raman methodologies. We are also part of a group sending a UV Raman instrument to Mars in 2020. I hear that there is a special one-way fare for spectroscopists for this measurement. We are also pioneering standoff UV Raman instruments for standoff trace explosive detection. ■

For more information on this topic, please visit our homepage at: [www.spectroscopyonline.com](http://www.spectroscopyonline.com)



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## PRODUCT INDEX

### NOS.

1,2-Dichloromethane	57
2,2,4-Trimethylpentane	57
3-D Visualization Software	59

### A

Accelerometers	63
Acetone	57
Acetonitrile	57
Acoustic Emission Analyzers	75
Acoustic Emission Equipment	63
Acousto-Optical Tunable Filter-Based Systems	32
Acousto-Optical Tunable Filters	45
AFM	40
Air Quality Monitors	73
Amino Acid Analyzers	79
Analog To Digital Converters	59
Analytical Standards/Reference Materials	50
Analyzer Enclosures/Housings/Shelters	76
Analyzers, Sensors and Testing Instruments	63
Applied Spectroscopic or Photometric Analyzers	70
Arc-Spark	22
Arc/Spark Spectrometers	70
Argon-Ion	44
Atmospheric Pressure Ionization	28
Atomic	36
Atomic	38
Atomic Absorption	22
Atomic Absorption Spectrometers	26
Atomic Absorption Spectrometers	40
Atomic Emission	22
Atomic Emission Spectrometers (including ICP & ICP-MS & DCP)	26
Atomic Emission Spectrometers (including ICP & ICP-MS & DCP)	40
Atomic Fluorescence	23
Atomic Force Microscopes	68
Atomic Spectroscopy	22
Atomic/Elemental Spectrometers	70

Attenuated Total Reflection/Internal Reflectance Cells	52
Attenuators	45
Auger	40
Automation Equipment	59
Autosamplers	59
Autosamplers	77

### B

Bag Sampling Devices	50
Balances	65
Barcode Sample Management Systems	59
Baseline Correction	59
Baths	65
Beam Optic Simulation Software	59
Beam Splitters	45
Benzene	57
Bioanalyzers and Related Equipment	77
Biosensors	77
BK7 Glass	58
Block Digestion Units, Programmable	52
Bolometers	63
Borosilicate Crown Glass	58
Butyl Acetate	57

### C

Calibration Equipment	64
Calibration Equipment/Services	76
Calibration Standards	50
Calorimeters	63
Calorimeters	75
Carbon Tetrachloride	57
CCD Cameras	67
CCD cameras/detectors	78
CCDs	41
CE-MS	27
Cell Positioning System	50
Centrifuges	65
Chart Recorders	59
Chemical Drawing	59
Chemical Ionization	28
Chemical Structure Software	59
Chemicals	64
Chemiluminescence Analyzers	75
Chemometrics Software	59
Chloroform	57
Chromatographic Process Analyzers	73
Chromatography, gas	77
Chromatography, ion	77
Chromatography, liquid	77
Chromatography, other	77
CIDs	41
CIDs	78
Circular Dichroism	35
Circular Dichroism (vibrational)	33
Circular Dichroism/Optical Rotary Dispersion Spectrometers	26
Circular Dichroism/Optical Rotary Dispersion Spectrometers	40
Clean Room Equipment	66
Clean Room Monitors	66
Closed Vessel	52
CO	44
CO <sub>2</sub>	44
Coherent Anti-Stokes Raman Spectroscopy (CARS)	33
Color Center	44
Colorimeters	26
Colorimeters	35
Colorimeters	40
Colorimeters	63
Colorimeters	70
Colorimeters	75
Colorimeters	75
Concentration/Density Analyzers	73
Concentric	54
Condition/Property Analyzers	73
Conductivity/pH/ORP	73
Confocal Microscopes	68
Consulting	62
Continuous Emissions Monitors	74
Contract Research & Analysis	62
CRDS	32

Crystal Optics	45
Crystalline Quartz	58
CT Scanning Equipment	63
CTDs	78
Cubic Zirconia	58
Cuvettes/Cells	50
Cyclohexane	57
Cylindrical Cells	51
Cylindrical Internal Reflectance	54

### D

Data Acquisition Boards	59
Data Acquisition Software	59
Data Acquisition/Handling Systems, Process	76
Data Management	59
Data Processing Software	59
Data Recorders	65
Data Subtraction	60
Dc Arc	43
Dedicated Data Stations	59
Densitometers	63
Densitometers	75
Derivatives	60
Detectors	29
Detectors & Related Equipment	41
Deuterium	43
Diamond	58
Diamond Anvil	54
Dichloromethane	57
Dielectric Analyzers	63
Diffuse Reflectance Cells	54
Digital Lock-In Amplifiers	41
Digital Signal Processors	59
Dilution Systems for Standard Preparation	50
Diode-Pumped Solid-State	44
Diode/Semiconductor	44
Dioxane	57
Direct Current Plasma Emission	22
Direct Injection	54
Discriminant Analysis	59
Dispersive Components (OEM)	42
Dispersive Infrared	30
Dispersive Raman	33
Distillation Systems	65
DNA Sequencing Equipment	79
Dosimeters	75
Double-Beam	35
Dye	44
Dynamic Mechanical Analyzers	63

### E

Eddy Current Equipment	63
EDS	40
Education/Training	62
Electron Ionization	28
Electronic Notebooks	60
Electrophoresis, capillary	77
Electrophoresis, gel	77
Electrophoresis, other	77
Electrospray	28
Electrospray Maximum Entropy Software	60
Electrothermal Vaporization	56
Elemental Analyzers	63
Elemental Mass Spectrometry	24
Ellipsometers	70
Employment Placement Firm	62
Enclosures	66
Energy-Dispersive XRF	24
Epoxyes or Polymers (Adhesives)	52
EPR	31
ESCA/X-Ray Photoelectron Spectroscopy	40
Ethanol (95 vol %)	57
Ethyl Acetate	57
Ethyl Formate	57
Ethyl Propionate	57
Evacuable Dies	52
Excimer	44

### F

Far-IR/Terahertz	29
Fence/Perimeter Monitoring Instruments	74
Fiber Optic Light Sources	43
Fiber Optics	67
Fiber Optics and Related Products	76
Fiber Optics, Mid-IR (bundles)	45
Fiber Optics, Mid-IR (single fibers)	46
Fiber Optics, Near-IR (bundles)	46
Fiber Optics, Near-IR (single fibers)	46
Fiber Optics, UV (single fibers)	46
Fiber Optics, UV (bundles)	46
Fiber-optic spectrophotometers	70
Field-Based Chromatography Equipment	74
Field-Based Spectroscopy Equipment	74
File Converters	60
Filter-Based Instruments	29
Filters/Filter Wheels	46
Filtration/Purification Equipment	65
Fittings/Flanges	65
Flame AA	22
Flame Photometers	70
Flint Glass (SF-10)	58
Flint Glass (SF-8)	58
Flooring	67
Flow Cells	51
Flow Injection Analysis	24
Flow injection analyzers	70
Flow Meters	63
Flow-Injection Analyzers	57
Flow-Through	54
Flowmeters	75
Fluid Handling Equipment	65
Fluorescence	29
Fluorescence	36
Fluorescence	38
Fluorescence Lifetime	30
Fluorescence Microscopes	68
Fluorescence Spectrometers	70
Fluorescence Spectrometers/Microplate Readers	26
Fluorescence Spectrometers/Microplate Readers	40
Fluorimeters	77
Fluxes, Fusions	52
Forensics/Illicit Drug Compounds	60
Fourier Transform Infrared (FT-IR)	30
Fourier Transform-IR Spectrometers	70
Fourier Transform-Near Infrared	32
FT-ICR-MS	27
FT-Raman	34
FT-Raman Accessories	54
Fume Hoods	67
Furniture	67

### G

GaAs	41
Gamma Counters	77
Gas	54
Gas Analyzers, Lab-Based	74
Gas Analyzers, Ambient	73
Gas Analyzers, Combustible	73
Gas Analyzers, On-Line	74
Gas Analyzers, Stack/Flue Emissions	74
Gas Analyzers, Toxic	74
Gas Chromatographs (GC), Process	73
Gas Generating Systems	64
Gases	64
GC-Infrared Spectrometers, Process	73
GC-IR	30
GC-IR analyzers	70
GC-Mass Spectrometers, Process	73
GC-MS	27
GC-MS analyzers	70
Ge	41
Gel Readers	79
Glassware	65
Glassware Washers	67
Glove Boxes	67



Gloves	67	Ion Mobility Spectrometers	71	Mass Spectrometry & Hyphenated Techniques	27	Near-IR Reflectance	32
Glow Discharge MS	24	Ion Selective Electrodes	63	Mass Spectrometry Detectors/ Electron Multipliers	41	Near-IR Spectrometers	71
Glow Discharge OES	22	Ion Trap MS	27	Matrix Assisted Laser Desorption Ionization (MALDI)	28	Near-IR Transmission	32
Glow-Discharge AA	22	Ion-Selective Electrodes	75	Mechanical Strength Testers	75	Nebulizers	54
Glycerol	57	Ionization Modes	27	Medical/In Vivo Diagnostics	36	Neutron Activation Analysis	24
Graphite Furnace	22	IR	36	Membrane Mirror Gratings	46	Nitrogen	44
Graphite Tubes	57	IR	37	Mercury Analyzers	22	NMR	36
Grinders	52	IR	60	Methacrylate	58	NMR	37
<b>H</b>		IR Arrays	41	Methanol	57	NMR	39
Halogen	43	IR Cards	52	Methyl Cyclohexane	57	NMR	61
Hardness Testing Equipment	63	IR Process Analyzers	30	Methyl Formate	57	NMR Imaging	31
Hardware	59	IRMS	24	Micro Cells	51	NMR Process Analyzers	31
Heaters/Coolers	65	Isooctane	57	Microanalysis/Imaging Equipment	40	NMR Spectrometers	26
Helium Cadmium	44	Isopropyl Alcohol	57	Microconcentric	54	NMR Spectrometers	40
Helium Neon	44	Isotopes, Radioactive	64	Microplate Readers	30	NMR Tubes	56
High Voltage Power Supplies	24	Isotopes, Stable	64	Microplate Readers	35	Non-Dispersive/Filter-Based Instruments	31
High Voltage Power Supplies	42	<b>K</b>		Microplate Readers	63	Nondestructive Testing Equipment	75
High Voltage Transformers, Custom & Standard Products	42	Krypton	43	Microplates, 1536-Well	78	Nondestructive Testing/ Inspection Equipment, General	63
High-Pressure	54	<b>L</b>		Microplates, 384-Well	78	Nondispersive IR Spectrometers	72
Hollow-Cathode	43	Labeled Compounds	50	Microplates, 96-Well	78	NSOM	40
Holographic Gratings	46	Labels and Labeling Equipment	76	Microplates, Other	78	Nuclear Magnetic Resonance Spectrometers	72
Holographic Notch Filters	46	Laboratory Chemicals, Gases and Materials	64	Microscope Accessories	67	Nucleic Acid Analyzers	79
Homogenizers	65	Laboratory Equipment	65	Microscopes	68	<b>O</b>	
Horizontal Attenuated Total Reflectance	54	Laboratory Equipment Repair	62	Microscopes, atomic force	79	OEM Modules & Instruments 500 V to 160 KV	43
Hotplates	52	Laboratory Furnishings	66	Microscopes, near-field scanning optical	79	On-Line Near-IR Analyzers For Process Analysis	33
HPLC/FT-IR Interfaces	52	Laboratory Information Management Systems	60	Microscopes, scanning electron	79	On-Line/At-Line/Near-Line Analyzers	38
Humidity Analyzers	74	Laboratory Presses	52	Microscopes, scanning tunneling	79	On-Line/Remote Analyzers	35
Hydride Generation	57	Lamps/Light Sources	43	Microscopes, confocal	79	Opacity/Turbidity Analyzers	75
Hyperspectral Imaging Equipment	74	Laser Ablation	57	Microscopes, Microspectrometers, and Imaging Equipment	67	Open-Path/Remote Sensing IR	31
Hyperspectral Imaging Equipment/ Software	67	Laser Alignment & Assorted Instruments	42	Microscopes, stereo	79	Open-Vessel	52
<b>I</b>		Laser Desorption	28	Microscopy Equipment (optical)	26	OPO	44
ICCDs	41	Laser Dyes	44	Microscopy Equipment (optical)	40	Optical Choppers	48
ICP-MS	23	Laser Induced Breakdown Spectrometers	71	Microscopy Equipment (SPM, SEM, TEM, STM, etc)	26	Optical Components/Fiber Optics	45
ICP-MS	24	Laser Power Meters/Probes	41	Microscopy Equipment (SPM, SEM, TEM, STM, etc)	40	Optical Crown Glass	58
ICP-MS Cones	57	Laser Safety Products	44	Microspectrometers	71	Optical Machinery	49
ICP-MS Systems	27	Laser-Based Analyzers	75	Microspectrometers, IR	79	Optical Remote Sensing Instruments	74
ICP, Axial	23	Laser-Induced Breakdown Spectroscopy (LIBS)	23	Microspectrometers, Raman	79	Optical Shutters	48
ICP, Combined Axial/Radial Capability	23	Lasers	26	Microspectroscopy	54	Optics	29
ICP, Radial	23	Lasers	40	Microwave Digestion/Extraction	52	Optodes	48
ICP, Sequential	23	Lasers	44	Microwave Spectrometers	71	Other	40
ICP, Simultaneous	23	LC-Infrared Spectrometers	73	Microwave-Assisted Extraction	52	Other	59
Image Analyzers/Intensifiers	67	LC-IR	31	Microwave-Induced Plasma Emission	23	Other	60
Image intensifiers	78	LC-Mass Spectrometers, Process	73	Microwell Plate Readers	54	Other Analyzers	63
Imaging	30	LC-MS	28	Mills	52	Other Atomic Techniques	24
Imaging analysis software	78	LED Lighting	43	Mirrors	46	Other Dispersive Components (OEM)	42
Imaging equipment, general	79	LIDAR	74	Miscellaneous Preparation Devices	52	Other Imaging Equipment/Accessories	67
Imaging Equipment/Accessories	67	Lighting	67	Mobile/Portable Laboratories	74	Other Industrial Analyzers and Testing Equipment	75
Imaging Systems	29	LIMS	59	Mobile/Portable/On-Site/Field-Based Analyzers	36	Other Instruments For Rent or Lease	27
Imaging/Microscopy/ Microanalysis Products	78	Liquid	54	Moisture Analyzers	74	Other Laboratory Chemicals, Gases and Materials	64
Immersion Probes	52	Liquid Analyzers, Lab-Based	74	Molecular Biology Instruments	79	Other Lamps/Light Sources	43
Immunoassays, automated	77	Liquid Analyzers, On-Line Moisture Analyzers	74	Molecular Modeling/Simulation	60	Other Lasers	44
Industrial Environmental Monitoring Instruments	74	Liquid Chromatographs (LC), Process	73	Molecular Spectroscopy	29	Other Medical/In Vivo Diagnostics	36
Industrial Hygiene Analyzers	74	Liquid Chromatography-Mass Spectrometers	77	Molecular Weight Analyzers	63	Other Microanalysis/Imaging Equipment	40
Infrared	44	Liquid Crystal Tunable Filters	46	Monochromators	42	Other Microscope Accessories	67
Infrared (mid-range)	30	Liquid Light Guides	46	MRI	31	Other Microscopes	69
Infrared (non-FT) Spectrometers	70	Liquid Scintillation Counters	77	MRI Testing Equipment	63	Other Miscellaneous Preparation Devices	52
Infrared Analyzers	75	Luminescence Spectrometers	71	MS	61	Other Mobile/Portable/On-Site/Field-Based Analyzers	37
Infrared Microscopes/ FT-IR Microspectrometers	68	Luminescence Spectrometers	77	MS (or GC-MS)	36	Other On-Line/At-Line/Near-Line Analyzers	39
Infrared Reflectance/Absorbance	30	<b>M</b>		MS (or GC-MS)	37	Other Optical Components/Fiber Optics	48
Infrared Spectrometers (including FT-IR & Near-IR)	26	Magnetic Resonance Imaging Systems	71	MS (or GC-MS)	38	Other Spectral Libraries	61
Infrared Spectrometers (including FT-IR & Near-IR)	40	Magnetic Resonance/NMR	31	Multichannel Plate Detectors	41	Oxygen Analyzers	74
Infrasil	58	Magnetic Sector Instruments	28	Multidimensional	31	<b>P</b>	
InGaAs	41	Magnetic Shielding	28	Multilayers	48	Partial Least Squares	59
Instrument Control Software	60	MALDI or MALDI -TOF	67	Multiplexers	48	Particle Analyzers, Lab-Based	75
Instrument Design	62	Mass Spectrometers	71	<b>N</b>		Particle Analyzers, On-Line	75
Instruments For Rent or Lease	26	Mass Spectrometers (including GC-MS, LC-MS & Mass Spectrometry Detectors)	40	N-Hexane	57	Particle Size Analyzers	63
Integrating Spheres	54	Mass Spectrometers (including GC-MS, LC-MS & Mass Spectrometry Detectors)	40	N,N-Dimethylformamide	57	Pb	41
Integration	60	Mass Spectrometry Detectors	40	Nd: YAG	44	PbS	41
Interferometers	42	Mass Spectrometry Detectors	40	Near-Field Scanning Microscopes	69	PbSe	41
Ion	44	Mass Spectrometry Detectors	40	Near-IR	32	PCR Systems	79
Ion Chromatographs (IC), Process	73	Mass Spectrometry Detectors	40	Near-IR	36	Peak Fitting	60
Ion Mobility	27			Near-IR	37		
				Near-IR	38		

Peak Picking	60	Raman Spectrometers	72	Spectrographs	42	Tunable Diode	45
Penetrometers	74	Reaction Monitors	31	Spectrometers	29	Tunable Dye	45
Petroleum Testing Equipment	75	Reagents	50	Spectrometers, IR	78	<b>U</b>	
PH Instruments	74	Reagents	65	Spectrometers, Mass	78	Ultra Fast	45
PH Instruments	75	Reference Materials and Certified		Spectrometers, NMR	78	Ultrasonic	56
pH Meters	63	Reference Materials, Inorganic	50	Spectrometers, other	78	Ultrasonic Testing Equipment	64
Pharmaceutical Compounds	61	Reference Materials and Certified		Spectrometers, Raman	78	Ultrasonic Testing Equipment	76
Photoacoustic	31	Reference Materials, Organic	50	Spectrometers, UV/Vis	78	UV Spectrometers	72
Photoacoustic	56	Reflectance	56	Spectrosil	58	UV-Grade Fused Silica	58
Photodiode Arrays	41	Refractometers	75	Specular Reflectance	56	UV-IR Lenses	49
Photoionization	28	Refractometers & Multi-Wave		Stable Isotopes	50	UV/Vis	35
Photometers	27	Length Analysis	64	Stack/Flue Gas Emissions Monitors	74	UV/Vis	36
Photometers	40	Refrigerators & Freezers	66	Standard Transmittance	51	UV/Vis	37
Photometers	63	Refrigerated/Previously Owned		Standards	65	UV/Vis	39
Photometers	72	Instruments	40	Statistical Process Control/ Quality Control Software	61	UV/Vis Spectrometers	72
Photometers	78	Remote/On-Line Raman Process		Step-Scan FT-IR Systems	31	UV/Vis Spectrophotometers	27
Photomicrographic Microscopes	69	Analyzers	34	Stereo Microscopes	69	UV/Vis Spectrophotometers	40
Photomultiplier Detectors	42	RF Generators, Solid State		STM	40	UV/Vis-Near-IR Analyzers	33
Pipettes	66	(27 & 40 MHz)	49	Stress/Strain Analyzers	75	UV/Vis-Near-IR Instruments	36
Plastic Ware	66	Rheology Equipment	64	Supercritical Fluid Chromatographs, Process	73	<b>V</b>	
Plate Readers	78	Robotics	59	Suprasil 300	58	Vacuum Equipment	66
Plate Readers, Spectrometers, Fluorescence	78	Round	51	Surface Analytical Instrumentation	27	Validation Software	60
Platinum Labware	52	<b>S</b>		Surface Analytical Instrumentation	40	Valves	66
Plumbing	67	Safety Equipment	76	Surface Analyzers	64	Valves, Fittings, Flanges	76
Pneumatic	56	Safety Equipment/Signage	67	Surface Spectroscopy & Microanalysis	40	Variable Temperature	56
Point-of-Measurement Analyzer Systems	36	Sample Conditioning Systems, Gas	76	Surface-Enhanced Raman Spectroscopy	34	Video Inspection Systems	67
Polarimeters	27	Sample Digestion Equipment/ Elemental Analysis	52	Synthesis Apparatus/Reactors	66	Video Monitors	67
Polarimeters	35	Sample Handling Accessories	52	Synthesis Equipment	79	Viscometers	64
Polarimeters	40	Sample Introduction Equipment	56	Synthetic Fused Silica	58	Viscometers	74
Polarimeters	64	Sapphire	58	Syringes	66	Viscometers	76
Polarimeters	75	Scanning Electron Microscopes	69	<b>T</b>		Visible Spectrometers	73
Polarization Optics	48	Scanning Probe Microscopes	69	Tanks	66	<b>W</b>	
Polarizing Microscopes	69	Scanning Tunneling Microscopes	69	TEM	40	Water	57
Polymer Compounds	61	SEM	40	Tempax	58	Water Purification Equipment	64
Polystyrene	58	Sensors	51	Temperature Control Devices	57	Water Quality Monitors	74
Principal Component Regression	59	Sensors, Chemical	75	Temperature/Pressure Controllers	66	Waveform Analyzers	76
Prisms	49	Sensors, Optical	75	Tensile Strength Analyzers	75	Wavelength-Dispersive XRF	24
Process Analytical Accessories/ Ancillary Products	76	Sensors, Other	75	Tensile Testing Equipment	64	Window/Cuvette Material Types	58
Professional Organization	62	SERS	40	Test and Measurement Equipment, General	76	Windows	49
Protective Clothing/Eyewear/Gloves	67	SFC-IR	31	Tetrachloroethylene	57	Workbenches	67
Proton-Induced Gamma Ray Emission	24	SFC-MS	31	Thermal Analyzers	76	<b>X</b>	
Proton-Induced X-Ray Emission	24	Shakers/Stirrers	66	Thermal Melt Analysis Accessories	57	X-Ray	36
Publishing	62	Shelving/Storage	67	Thermogravimetric Analyzers	64	X-Ray	38
Pumps	66	Silicon Diodes/Photocells	42	Thermogravimetric Analyzers-Infrared Spectrometers	72	X-Ray	39
Purge-and-Trap Devices	73	SIMS	28	Thermogravimetric Analyzers-Mass Spectrometers	72	X-Ray	43
Purification Equipment	79	SIMS	40	Thermomechanical Analyzers	64	X-ray Analysis Equipment	76
Pyrex	58	Simultaneous Digestion Systems	52	Thin Film Fabricators	52	X-ray Diffraction	24
Pyrolysis Equipment	64	Single-Beam	35	Thin-Layer Chromatography, Process	73	X-Ray Diffractometers	27
Pyrolyzers	52	Slides and Mounts	68	Threaded Cap	52	X-Ray Diffractometers	40
<b>Q</b>		Smoothing	60	Ti: Sapphire	45	X-Ray Fluorescence Spectrometers	27
Quadrupole Instruments	28	Sodium Chloride	58	Time Resolved	30	X-Ray Fluorescence Spectrometers	40
Quantitation	60	Software	59	TIMS	24	X-ray Microanalysis/Imaging	24
Quartz Tungsten-Halogen	43	Software	68	Tip-Enhanced Raman Spectroscopy	35	X-Ray Optics	49
Quartz, Extremely Low O-H	58	Software, Chemometrics	76	Titration	61	X-ray Spectrometers	
<b>R</b>		Software, Instrument Control	76	TOC-CRDS	34	(Energy-Dispersive)	73
Radiometers	64	Software, Validation	76	TOF-MS	28	X-ray Spectrometers	
Raman	36	Solid	56	Toluene	57	(Wavelength-Dispersive)	73
Raman	37	Solid-State	31	Total Reflection XRF	24	X-Ray Spectrometry	24
Raman	39	Solids/Slurries Analyzers, Lap-Based	74	Training/Tutorial Programs	60	Xenon	43
Raman	61	Solids/Slurries Analyzers, On-Line	74	Transflectance	56	Xylene	57
Raman & Related		Solvents	57	Transmission	56	<b>Z</b>	
Vibrational Techniques	33	Solvents	65	Transmission Electron Microscopes	69	Zeeman	22
Raman Microscopes/ Microspectrometers	69	Sources (lasers, other)	29	Trimethyl Phosphate	57		
Raman Microspectroscopy/ Raman Imaging	34	Spark Ablation	57	Tubing	66		
Raman Spectrometers	27	Specimen Preparation	68				
Raman Spectrometers	40	Spectral Interpretation	62				
		Spectral Libraries	60				
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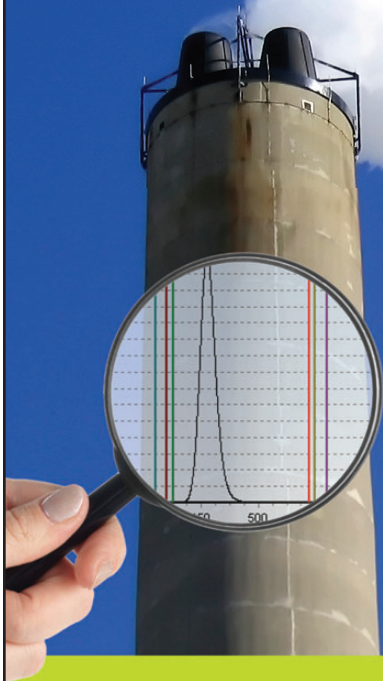


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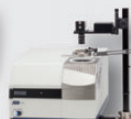
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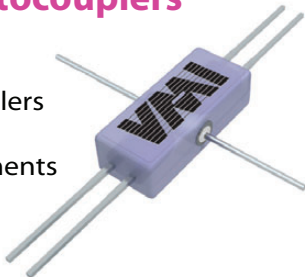
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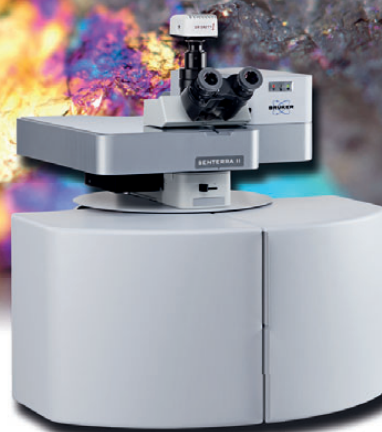
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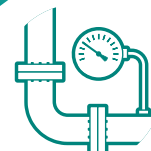
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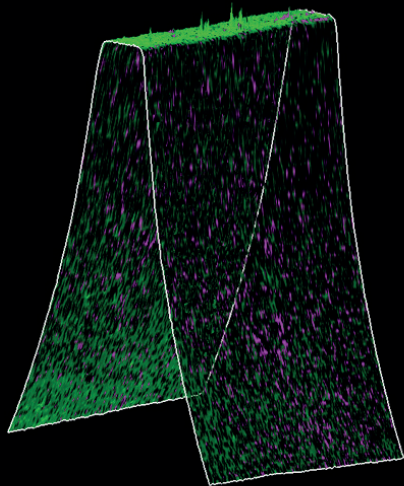


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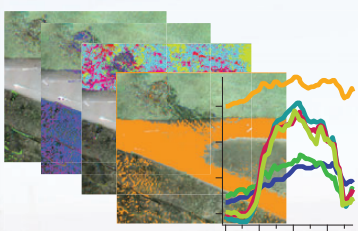

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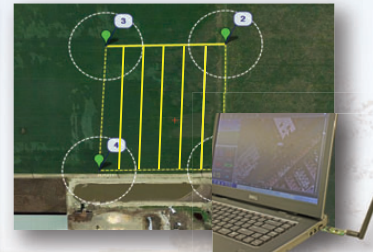


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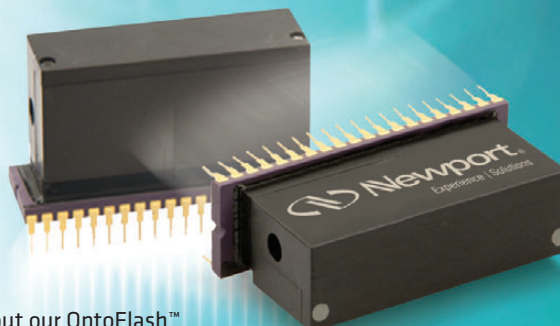
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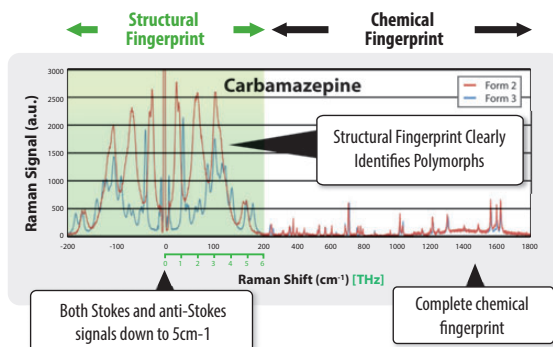
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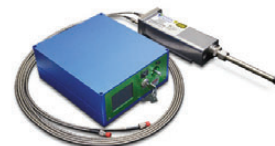
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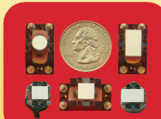
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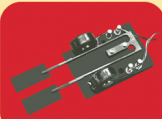
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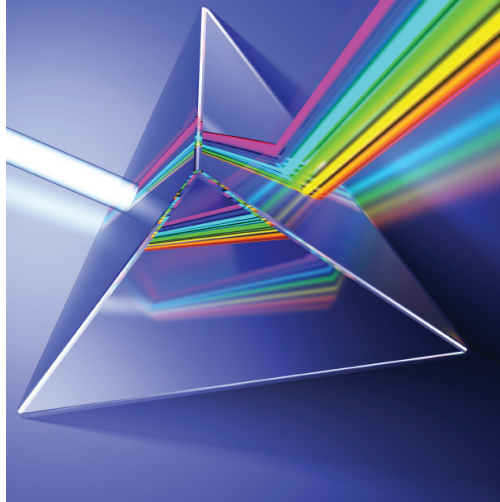
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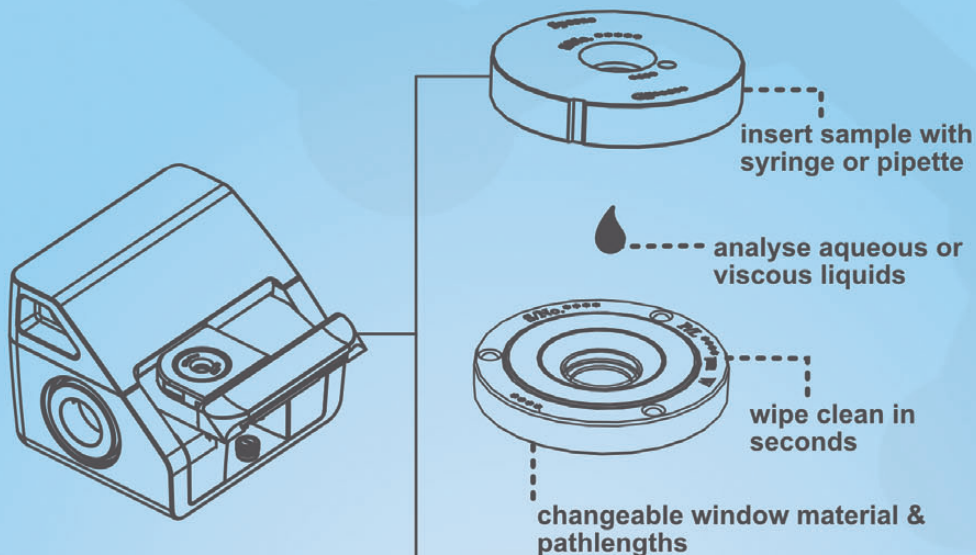
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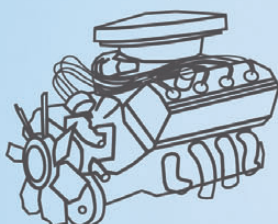
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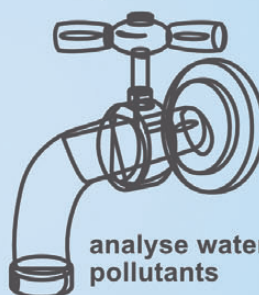
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# A Breakthrough in IR & Raman Spectral Identification

**ON-DEMAND WEBINAR** Aired July 20, 2016

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Scientists using spectroscopy to identify unknown compounds need the right answers, and they need them quickly. This webinar introduces the latest technologies to identify unknown IR and Raman spectra and the advantages it has over traditional tools.

- See live identifications of real spectral samples, including complex mixtures.
- Learn about a patent-pending technology that applies multiple spectral corrections to compensate for differences between spectra caused by variability of instruments, accessories, and other factors, including human error.
- Review studies that reveal the impact of this technology on spectral identification as compared to traditional spectral search.

**Who Should Attend:**

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**Gregory M. Banik,  
Ph.D., V.S.M.**  
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**Key Learning Objectives:**

- How to increase the efficiency and accuracy of spectral identification
- How to optimize results by combining high-quality reference spectral data with superior software technology
- How to use turnkey technologies so experts and non-experts alike can identify unknown spectra with confidence

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For questions, contact Kristen Moore at [kmoore@advanstar.com](mailto:kmoore@advanstar.com)



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Lenox Laser Corp  
Parker Balston  
Filtration & Separation Div,  
Parker Hannifin Corp  
SCINCO CO., LTD

## GASES

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Campro Scientific GmbH  
CEA Instruments  
Icon (Isotope) Services  
MIL-RAM Technology  
Parker Balston  
Filtration & Separation Div,  
Parker Hannifin Corp  
Peak Scientific

## ISOTOPES, RADIOACTIVE

American Radiolabeled Chemicals  
Berkeley Nucleonics Corp  
Campro Scientific GmbH

## ISOTOPES, STABLE

American Radiolabeled Chemicals  
C/D/N Isotopes  
Cambridge Isotope Labs  
Campro Scientific GmbH  
Cerilliant Corp  
High-Purity Standards  
Icon (Isotope) Services  
Pfaltz & Bauer  
SPEX CertiPrep  
VHG Labs/LGC Standards

## OTHER LABORATORY CHEMICALS, GASES AND MATERIALS

Accumet Materials Co  
Accurate Chemical and Scientific Corp  
**Agilent Technologies**  
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800-227-8770  
Cambridge Isotope Labs  
Claisse Scientific Corp  
**GFS Chemicals**  
740-817-5825  
Ladd Research Industries  
Parker Balston  
Filtration & Separation Div,  
Parker Hannifin Corp  
Sierra Instruments

Soltec Ventures  
SPEX CertiPrep  
WA Hammond Drierite Co  
Worthington Biochemical Corp

## REAGENTS

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Burrell Scientific  
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Campro Scientific GmbH  
Cerilliant Corp  
Claiss Scientific Corp  
Crescent Chemical Co  
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Electron Microscopy Sciences  
EMS Acquisition Corp

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High-Purity Standards  
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### Inorganic Ventures

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Pfaltz & Bauer  
Premier Lab Supply  
Qorpak  
SCIEX  
Soltec Ventures  
SPEX CertiPrep  
VHG Labs/LGC Standards  
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## STANDARDS

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ASI Standards  
Avian Technologies  
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Texas Scientific Products  
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## LABORATORY EQUIPMENT

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Ladd Research Industries  
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Qorpak  
Scientech

### Shimadzu Scientific Instruments

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www.ssi.shimadzu.com  
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800-477-1227

Terriss Consolidated Industries  
Tomopal

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Brookfield AMETEK  
Instrumentation & Specialty Controls  
Capovani Brothers  
Denville Scientific  
HEMCO Corp  
Kewaunee Scientific Corp  
Leedal Mfg Group  
Leedal  
Omega Engineering  
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EMS Acquisition Corp  
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Ladd Research Industries  
Nuaire  
PRO Scientific  
Sarstedt

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952-935-4100  
USA Scientific  
Wilmaad-LabGlass  
World Precision Instruments

### DATA RECORDERS

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Denville Scientific  
GrayWolf Sensing Solutions  
Hampshire Controls Corp  
Industrial Test Systems  
Omega Engineering  
Pentek

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Andrews Glass Co  
Denville Scientific  
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NexGen Enviro Systems

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SCP SCIENCE  
Seal Analytical  
SPEX CertiPrep  
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Wheaton Science Products

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SPEX CertiPrep  
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Kewaunee Scientific Corp  
Materion Electrofusion  
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Parker Hannifin  
Precision Fluidics  
Qosina  
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UVP LLC  
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Ladd Research Industries  
LaMotte Co  
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Qosina  
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952-935-4100

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Texas Scientific Products  
USA Scientific  
Wheaton Science Products

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AutoMate Scientific  
Braintree Scientific  
Busch LLC  
Clark Solutions  
Cole-Parmer Instrument Co  
Colfax Fluid Handling  
Zenith  
Duniway Stockroom Corp  
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Parker Hannifin  
Precision Fluidics  
Seal Analytical  
Tek Temp Instruments  
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Vindum Engineering  
Walchem IWAKI AMERICA  
Wheaton Science Products  
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PRO Scientific  
Qorpak  
Sarstedt  
Tomopal  
USA Scientific  
Verder Scientific  
Retsch  
Wheaton Science Products

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Denville Scientific  
Harvard Apparatus  
P J Cobert Assocs  
Parker Hannifin  
Precision Fluidics  
Qorpak  
Qosina  
Qosmedix  
**Spectral Systems**  
Ted Pella  
Tomopal  
Wheaton Science Products  
Wilmad-LabGlass  
Wyatt Technology Corp

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Leedal Mfg Corp  
Leedal  
Tek Temp Instruments

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AABSPEC Instrumentation Corp  
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AutoMate Scientific  
Braintree Scientific  
Brooks Instrument  
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Vacuum Research Corp  
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Inotech Bioscience, LLC  
Intellitech  
Metal Technology  
P J Cobert Assocs  
Parker Hannifin  
Precision Fluidics  
Qorpak  
Qosina  
Qosmedix  
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## VACUUM EQUIPMENT

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Capovani Brothers  
Cryo Industries of America  
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MKS Instruments  
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Sierra Instruments  
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Vacuum Research Corp  
Vat  
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Advanced Specialty Gas Equipment  
AutoMate Scientific  
Brooks Instrument  
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MKS Instruments  
Omega Engineering  
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Filtration & Separation Div,  
Parker Hannifin Corp  
Parker Hannifin  
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Peter Paul Electronics Co  
Qosina  
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Tomopal  
Vacuum Research Corp  
Vat  
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## LABORATORY FURNISHINGS

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Carbolite

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ENMET  
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Qorpak  
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Leedal Mfg Group  
Leedal  
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MicroImage Video Systems  
New England Photoconductor  
PHOTONIS  
Scientific Detectors  
Piezosystem Jena GmbH  
Prior Scientific  
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Carltext  
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ACCESSORIES**Accu-Scope  
Advanced Imaging Concepts  
Aerotech  
Applied Image  
Bangs Labs  
Bel-Art - SP Scienceware  
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Cryo Industries of America  
Denville Scientific  
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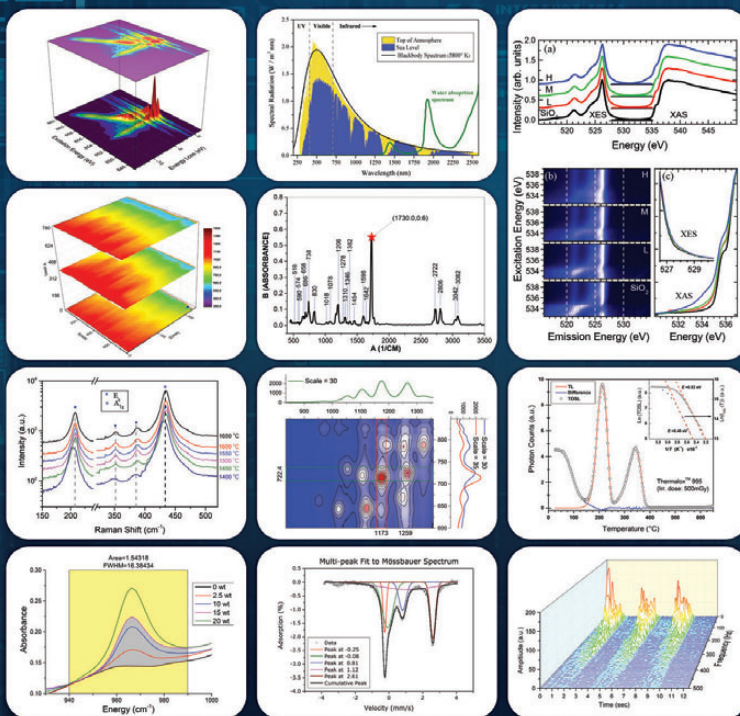
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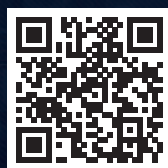
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- the types of data and samples they collected under challenging conditions during the mission
- how the analysis of their valuable samples in the field accelerates scientific discoveries
- what Isotope Ratio Infrared Spectroscopy contributed to the success of the mission

**Key Learning Objectives:**

- Learn about the Trail by Fire mission and the cutting edge volcano research it represents
- Learn about the benefits of field-based analysis with isotope ratio infrared spectrometers
- Discover how you can take home results instead of samples

For questions, contact Kristen Moore at [kmoore@advanstar.com](mailto:kmoore@advanstar.com)

**Presenter:**

**Dr. C. Ian Schipper**  
Lecturer, Igneous Processes  
Victoria University  
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**Moderator:**  
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**Who Should Attend:**

- Scientists interested in environmental analysis and isotope ratio analysis
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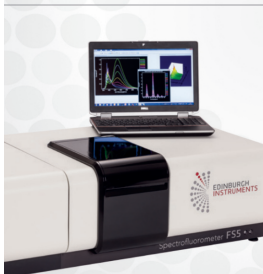
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**JM Science**  
SCINCO CO., LTD  
Tomopal

Wyatt Technology Corp

### PURGE-AND-TRAP DEVICES

AABSPEC Instrumentation Corp  
CDS Analytical  
INFICON  
OI Analytical

### SUPERCritical FLUID CHROMATOGRAPHS, PROCESS

AABSPEC Instrumentation Corp  
**Agilent Technologies**  
**Life Sciences & Chemical Analysis**  
800-227-8770

### THIN-LAYER CHROMATOGRAPHY, PROCESS

**Agilent Technologies**  
**Life Sciences & Chemical Analysis**  
800-227-8770  
Miles Scientific (Analtech)  
UVP LLC

### CONDITION/PROPERTY ANALYZERS

### AIR QUALITY MONITORS

CDS Analytical  
CEA Instruments  
Control Instruments Corp  
Daylight Solutions

ENMET  
Environmental Devices Corp  
Extrel CMS  
GrayWolf Sensing Solutions  
HEMCO Corp  
**HORIBA Scientific**  
INFICON  
IRSweep AG  
Laser Components USA  
Mesa Labs  
MIL-RAM Technology  
MKS Instruments  
PACS Courses & Conferences,  
Training & Testing  
Sensor Electronics Corp

### CONCENTRATION/DENSITY ANALYZERS

**Agilent Technologies**  
**Life Sciences & Chemical Analysis**  
800-227-8770  
Environmental Devices Corp  
Laser Components USA

### CONDUCTIVITY/PH/ORP

Industrial Test Systems  
OI Analytical  
Omega Engineering  
optek-Danulat

### GAS ANALYZERS, AMBIENT

ABB  
Analytical Measurementation  
CEA Instruments  
Control Instruments Corp  
Emerson Process Mgmt  
Rosemount  
ENMET  
Environmental Devices Corp  
Extrel CMS  
GrayWolf Sensing Solutions  
INFICON  
International Crystal Labs  
IRSweep AG  
LI-COR  
MIL-RAM Technology  
MKS Instruments  
MKS Instruments  
OI Analytical  
Sensor Electronics Corp  
**Thermo Scientific - Molecular Spectroscopy**  
**Part of Thermo Fisher Scientific**  
800-532-4752  
Tiger Optics LLC

### GAS ANALYZERS, COMBUSTIBLE

**Agilent Technologies**  
**Life Sciences & Chemical Analysis**  
800-227-8770  
CEA Instruments  
Control Instruments Corp  
Emerson Process Mgmt  
Rosemount  
ENMET  
Environmental Devices Corp  
Extrel CMS  
Idealab  
INFICON  
IRSweep AG  
MIL-RAM Technology  
Sensor Electronics Corp  
Spectraline  
Instrument Div  
**Thermo Scientific - Molecular Spectroscopy**  
**Part of Thermo Fisher Scientific**  
800-532-4752

**GAS ANALYZERS, LAB-BASED**

**ABB Analytical Measurement**  
800-858-3847

**Agilent Technologies**  
**Life Sciences & Chemical Analysis**  
800-227-8770

Burrell Scientific  
Extrel CMS  
INFICON  
International Crystal Labs

IRsweep AG  
LI-COR  
MEECO

OI Analytical

**Simplex Scientific**  
808-831-4476

**Thermo Scientific - Molecular Spectroscopy**  
**Part of Thermo Fisher Scientific**  
800-532-4752

Tiger Optics LLC

**GAS ANALYZERS, ON-LINE**

ABB  
Analytical Measurement  
**ABB Analytical Measurement**  
800-858-3847

CEA Instruments  
Control Instruments Corp  
Extrel CMS

INFICON  
Kaiser Optical Systems

LaVision GmbH  
MEECO

MIDAC Corp  
MKS Instruments

**Simplex Scientific**  
808-831-4476

**Thermo Scientific - Molecular Spectroscopy**  
**Part of Thermo Fisher Scientific**  
800-532-4752

Tiger Optics LLC

**GAS ANALYZERS, STACK/FLUE EMISSIONS**

ABB  
Analytical Measurement  
**Agilent Technologies**

**Life Sciences & Chemical Analysis**  
800-227-8770

Applied Analytics  
CEA Instruments  
Control Instruments Corp  
Emerson Process Mgmt

Rosemount  
Environmental Devices Corp  
Extrel CMS

Idealab  
MIDAC Corp  
MIL-RAM Technology

MKS Instruments  
optek-Danulat

**Savillex Corp**  
952-935-4100

**Thermo Scientific - Molecular Spectroscopy**  
**Part of Thermo Fisher Scientific**  
800-532-4752

Tiger Optics LLC

**GAS ANALYZERS, TOXIC**

**Agilent Technologies**  
**Life Sciences & Chemical Analysis**  
800-227-8770

CEA Instruments  
Control Instruments Corp  
Emerson Process Mgmt

Rosemount  
ENMET

Environmental Devices Corp  
Extrel CMS

GrayWolf Sensing Solutions  
Idealab  
INFICON

IRsweep AG  
Laser Components USA  
MIDAC Corp

MIL-RAM Technology  
MKS Instruments  
OI Analytical

**Savillex Corp**  
952-935-4100

Sensor Electronics Corp  
Spectraline  
Instrument Div

**Thermo Scientific - Molecular Spectroscopy**  
**Part of Thermo Fisher Scientific**  
800-532-4752

**HUMIDITY ANALYZERS**

Elan Technical Corp  
Environmental Devices Corp  
GrayWolf Sensing Solutions

MEECO  
Omega Engineering  
Sensor Electronics Corp  
Tiger Optics LLC

**LIQUID ANALYZERS, LAB-BASED**

**Agilent Technologies**  
**Life Sciences & Chemical Analysis**  
800-227-8770

IRsweep AG  
Laser Components USA  
LT Industries

Wyatt Technology Corp

**LIQUID ANALYZERS, ON-LINE MOISTURE ANALYZERS**

Guided Wave  
LT Industries

**MOISTURE ANALYZERS**

**CEM Corp**  
J&M Analytik AG  
**JM Science**

Laser Components USA  
LI-COR  
MEECO

Tiger Optics LLC

**OXYGEN ANALYZERS**

**Agilent Technologies**  
**Life Sciences & Chemical Analysis**  
800-227-8770

CEA Instruments  
Control Instruments Corp  
ENMET

getSpec.com  
GrayWolf Sensing Solutions  
**HORIBA Scientific**

LaMotte Co  
Laser Components USA  
MIL-RAM Technology

Tiger Optics LLC

**PH INSTRUMENTS**

Analytical Measurements  
Dakota Instruments  
Industrial Test Systems

LaMotte Co

**Ocean Optics**  
727-733-2447

OI Analytical  
Omega Engineering

**SOLIDS/SLURRIES ANALYZERS, LAP-BASED**

Applied Analytics  
**CEM Corp**  
LT Industries  
LTB Lasertechnik Berlin GmbH

**SOLIDS/SLURRIES ANALYZERS, ON-LINE**

Applied Analytics  
LT Industries  
LTB Lasertechnik Berlin GmbH  
optek-Danulat  
Process Instruments  
SPECTRO Analytical Instruments  
Div of Ametek

**VISCOMETERS**

Burrell Scientific  
Premier Lab Supply  
Process Instruments  
Scantek  
Spectro Scientific  
Stony Brook Scientific Ltd  
**Thermo Scientific - Molecular Spectroscopy**  
**Part of Thermo Fisher Scientific**  
800-532-4752

**INDUSTRIAL ENVIRONMENTAL MONITORING INSTRUMENTS****CONTINUOUS EMISSIONS MONITORS**

Control Instruments Corp  
Environmental Devices Corp  
Extrel CMS

INFICON

IRsweep AG

LI-COR

MIDAC Corp

MIL-RAM Technology

MKS Instruments

OI Analytical

optek-Danulat

Sierra Instruments

**Thermo Scientific - Molecular Spectroscopy**

**Part of Thermo Fisher Scientific**  
800-532-4752

US Nuclear Corp

Technical Assocs

**FENCELINE/PERIMETER MONITORING INSTRUMENTS**

Environmental Devices Corp

Extrel CMS

INFICON

MIDAC Corp

MIL-RAM Technology

**FIELD-BASED CHROMATOGRAPHY EQUIPMENT**

**Agilent Technologies**  
**Life Sciences & Chemical Analysis**  
800-227-8770

INFICON

**FIELD-BASED SPECTROSCOPY EQUIPMENT**

**Agilent Technologies**  
**Life Sciences & Chemical Analysis**  
800-227-8770

Artel

DSP Instruments

Ibsen Photonics

MIDAC Corp

XIA LLC

XOS

**HYPERSPECTRAL IMAGING EQUIPMENT**

En'Urga  
inno-spec GmbH

Optronic Labs LLC  
DBA Gooch & Housego  
P&P Optica  
Spectraline  
Instrument Div  
Telops  
Tornado Spectral Systems  
Wasatch Photonics

**INDUSTRIAL HYGIENE ANALYZERS**

ENMET  
Environmental Devices Corp  
GrayWolf Sensing Solutions  
INFICON  
MIL-RAM Technology

**LIDAR**

Daylight Solutions  
Laser Components USA  
UTC Aerospace Systems  
Sensors Unlimited, Products

**MOBILE/PORTABLE LABORATORIES**

**Agilent Technologies**  
**Life Sciences & Chemical Analysis**  
800-227-8770

DSP Instruments

INFICON

**OPTICAL REMOTE SENSING INSTRUMENTS**

**Agilent Technologies**  
**Life Sciences & Chemical Analysis**  
800-227-8770

Daylight Solutions  
DSP Instruments  
Environmental Devices Corp

Ibsen Photonics

IRsweep AG

Laser Components USA

LT Industries

MIDAC Corp

Omega Engineering

OZ Optics Ltd

PLX

Telops

Tornado Spectral Systems

Ushio America

UTC Aerospace Systems  
Sensors Unlimited, Products

**PENETROMETERS**

Stony Brook Scientific Ltd

**STACK/FLUE GAS EMISSIONS MONITORS**

CEA Instruments  
Environmental Devices Corp  
MIL-RAM Technology

MKS Instruments

optek-Danulat

**Savillex Corp**

952-935-4100

Sierra Instruments

**WATER QUALITY MONITORS**

Cecil Instruments Ltd

Extrel CMS

Horizon Technology

Industrial Test Systems

INFICON

LaMotte Co

Lovibond Tintometer

MIL-RAM Technology

OI Analytical

optek-Danulat

PACS Courses & Conferences,

Training & Testing

Spectraline

Instrument Div

SPECTRO Analytical Instruments  
Div of Ametek  
Turner Designs  
US Nuclear Corp  
Technical Assess  
XOS

## OTHER INDUSTRIAL ANALYZERS AND TESTING EQUIPMENT

### ACOUSTIC EMISSION ANALYZERS

Scantek

### CALORIMETERS

Control Instruments Corp  
LECO Corp  
Mettler-Toledo  
**PerkinElmer**  
Analytical Sciences  
203-925-4600

Sciencetech  
SCINCO CO., LTD

### CHEMILUMINESCENCE ANALYZERS

BMG LABTECH GmbH  
Emerson Process Mgmt  
Rosemount  
PicoQuant GmbH

### COLORIMETERS

Bel-Art - SP Scienceware  
Industrial Test Systems  
J&M Analytik AG  
LaMotte Co  
Lovibond Tintometer  
SCINCO CO., LTD  
Seal Analytical  
Westboro Photonics

### DENSITOMETERS

UVP LLC

### DOSIMETERS

Berkeley Nucleonics Corp  
Environmental Devices Corp  
MIL-RAM Technology  
S E Intl

### FLOWMETERS

Aalborg Instruments  
Acromag  
Advanced Specialty Gas Equipment  
Applied Analytics  
Brooks Instrument  
Clark Solutions  
CONCOA/Controls Corp America  
Dakota Instruments  
Exair Corp  
GrayWolf Sensing Solutions  
MKS Instruments  
Omega Engineering  
Sierra Instruments

### INFRARED ANALYZERS

ABB  
Analytical Measurementation

**ABB Analytical Measurement**  
Email: fitir@ca.abb.com  
www.abb.com/analytical  
fax 418-877-2834  
800-858-3847

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Applied Analytics  
Control Instruments Corp  
Daylight Solutions  
DSP Instruments  
Environmental Devices Corp  
Idealab  
International Crystal Labs  
IRsweep AG

LI-COR  
LT Industries  
MIL-RAM Technology  
New England Photoconductor

### PerkinElmer

Analytical Sciences  
Email: customercareus@perkinelmer.com  
www.perkinelmer.com  
203-925-4600

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Sensor Electronics Corp

**Simplex Scientific**  
608-831-4476

**Thermo Scientific - Molecular Spectroscopy**

**Part of Thermo Fisher Scientific**  
800-532-4752

UTC Aerospace Systems  
Sensors Unlimited, Products

### ION-SELECTIVE ELECTRODES

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770

Analytical Measurements  
Exair Corp  
LaMotte Co

### LASER-BASED ANALYZERS

Block Engineering  
Brookhaven Instruments Corp  
Coherent  
Daylight Solutions  
Fritsch GmbH  
Milling and Sizing  
**HORIBA Scientific**  
Industrial Test Systems  
Laser Components USA  
LTB Lasertechnik Berlin GmbH  
Process Instruments  
Tiger Optics LLC

### MECHANICAL STRENGTH TESTERS

NSL Analytical Services  
Quad Group

### NONDESTRUCTIVE TESTING EQUIPMENT

#### AMPTEK

Email: sales@amptek.com  
www.amptek.com  
fax 781-275-3470  
781-275-2242

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Block Engineering

#### EDAX

**Materials Analysis Div**  
800-535-3329

**HORIBA Scientific**

Kugler of America Ltd  
LT Industries  
Micro Photonics  
Spellman High Voltage Electronics Corp

**Thermo Scientific - Molecular Spectroscopy**

**Part of Thermo Fisher Scientific**  
800-532-4752

Tornado Spectral Systems  
TREK  
Wasatch Photonics

### OPACITY/TURBIDITY ANALYZERS

Artel  
SCINCO CO., LTD

### PARTICLE ANALYZERS, LAB-BASED

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770

#### AMPTEK

781-275-2242  
Angstrom-Advanced  
Brookhaven Instruments Corp  
Fritsch GmbH  
Milling and Sizing  
**HORIBA Scientific**  
Malvern Instruments  
Mettler-Toledo  
NSL Analytical Services  
Spectro Scientific

### PARTICLE ANALYZERS, ON-LINE

Brookhaven Instruments Corp  
Environmental Devices Corp  
Malvern Instruments  
Mettler-Toledo  
Wyatt Technology Corp

### PETROLEUM TESTING EQUIPMENT

**ABB Analytical Measurement**  
800-858-3847

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770

Brookfield AMETEK  
Instrumentation & Specialty Controls  
Eastern Applied Research  
Guided Wave  
**Thermo Scientific - OES & X-Ray Analyzers**  
**Part of Thermo Fisher Scientific**  
Tornado Spectral Systems  
XOS

### PH INSTRUMENTS

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770

Analytical Measurements  
getSpec.com  
Industrial Test Systems  
LaMotte Co

#### Ocean Optics

Email: info@oceanoptics.com  
www.oceanoptics.com  
fax 727-733-3962  
727-733-2447

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Omega Engineering

### POLARIMETERS

Glas-Col  
PDR-Chemical LLC  
**PerkinElmer**  
**Analytical Sciences**  
203-925-4600  
Rudolph Instruments dba DigiPol  
Technologies

### REFRACTOMETERS

Rudolph Instruments  
dba DigiPol Technologies  
Terriss Consolidated Industries  
Wyatt Technology Corp

### SENSORS, CHEMICAL

Applied Analytics  
Block Engineering  
Control Instruments Corp  
ENMET  
GrayWolf Sensing Solutions  
Laser Components USA  
MIL-RAM Technology  
PACS Courses & Conferences,  
Training & Testing

Process Instruments  
Walchem IWAKI AMERICA

### SENSORS, OPTICAL

AIA - Advanced Vision + Imaging  
art photonics GmbH  
Carl Zeiss Spectroscopy GmbH  
Daylight Solutions  
DSP Instruments

**Edinburgh Instruments**  
Photonics

+44-1506-425-300  
Electro Optical Systems  
Environmental Devices Corp  
Gentec Electro-Optics  
getSpec.com  
Hamamatsu Photonics UK Ltd  
Irradian Ltd  
IRsweep AG  
ITF Technologies  
J&M Analytik AG  
Laser Components USA  
LaVision GmbH  
LT Industries  
New England Photoconductor

#### Ocean Optics

Email: info@oceanoptics.com  
www.oceanoptics.com  
fax 727-733-3962  
727-733-2447

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Omega Engineering  
OZ Optics Ltd  
Photek Ltd  
PHOTONIS  
Scientific Detectors  
Sciencetech  
Selex ES Ltd  
Solar Light Co  
UTC Aerospace Systems  
Sensors Unlimited, Products  
UVP LLC

### SENSORS, OTHER

Acromag  
CEA Instruments  
**Edinburgh Instruments**  
Photonics  
+44-1506-425-300  
Elan Technical Corp  
Environmental Devices Corp  
Laser Components USA  
MIL-RAM Technology  
New England Photoconductor

#### Ocean Optics

727-733-2447  
Omega Engineering  
Photek Ltd  
PHOTONIS  
Scientific Detectors  
S-Products  
Selex ES Ltd  
Sierra Instruments  
TREK

### STRESS/STRAIN ANALYZERS

Biodata Ltd  
Electro Standards Labs  
Omega Engineering  
**PerkinElmer**  
**Analytical Sciences**  
203-925-4600  
Quad Group  
Rudolph Instruments  
dba DigiPol Technologies  
Windmill Software Ltd

### TENSILE STRENGTH ANALYZERS

Brookfield AMETEK  
Instrumentation & Specialty Controls  
NSL Analytical Services



**PerkinElmer**  
Analytical Sciences  
203-925-4600

Quad Group

## TEST AND MEASUREMENT EQUIPMENT, GENERAL

Aerotech  
**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770

Applied Analytics  
Applied Image  
Artel  
Berkeley Nucleonics Corp  
Biodata Ltd  
Brookfield AMETEK  
Instrumentation & Specialty Controls  
Brooks Instrument  
Burrell Scientific

CEA Instruments  
Eastern Applied Research  
**Edinburgh Instruments**  
Photonics

+44-1506-425-300

Fischer Technology  
Gentec Electro-Optics  
GrayWolf Sensing Solutions  
Hampshire Controls Corp  
**HORIBA Scientific**  
Industrial Test Systems  
LaMotte Co  
LT Industries

Malvern Instruments  
Micro Photonics  
MicroImage Video Systems  
MIL-RAM Technology  
NSL Analytical Services  
Omega Engineering  
Optronic Labs LLC  
DBA Gooch & Housego  
OZ Optics Ltd  
Pentek  
Piezosystem Jena GmbH  
Prior Scientific  
Quad Group  
Sierra Instruments  
Terahertz Technologies  
TREK  
Unitron Ltd  
Windmill Software Ltd

## THERMAL ANALYZERS

AABSPEC Instrumentation Corp  
DSP Instruments  
Omega Engineering

**PerkinElmer**  
Analytical Sciences  
203-925-4600  
SCINCO CO., LTD

## ULTRASONIC TESTING EQUIPMENT

Exair Corp  
Micro Photonics  
Reynard Corp

## VISCOMETERS

Brookfield AMETEK  
Instrumentation & Specialty Controls  
Burrell Scientific  
Malvern Instruments

**PerkinElmer**  
Analytical Sciences  
203-925-4600

Scantek  
Stony Brook Scientific Ltd  
**Thermo Scientific - Molecular Spectroscopy**  
Part of Thermo Fisher Scientific  
800-532-4752  
Vindum Engineering

## WAVEFORM ANALYZERS

Berkeley Nucleonics Corp

## X-RAY ANALYSIS EQUIPMENT

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770

### AMPTEK

Email: sales@amptek.com  
www.amptek.com  
fax 781-275-3470  
781-275-2242

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Cianflone Scientific Instruments Corp  
Eastern Applied Research

### EDAX

Materials Analysis Div  
Email: info.edax@ametec.com  
www.edax.com  
fax 201-529-3156  
800-535-3329

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Fischer Technology  
**HORIBA Scientific**  
IfG - Institute for Scientific  
Instruments GmbH

Inel  
Lenox Laser Corp  
Micro Photonics  
PACS Courses & Conferences,  
Training & Testing  
Princeton Gamma-Tech Instruments

### Rigaku

S E Intl  
SGX Sensortech (MA) Ltd  
SPECTRO Analytical Instruments  
Div of Ametek

**Thermo Scientific - OES & X-Ray Analyzers**

Part of Thermo Fisher Scientific  
VHG Labs/LGC Standards  
XIA LLC  
XOS

## PROCESS ANALYTICAL ACCESSORIES/ANCILLARY PRODUCTS

## ANALYZER ENCLOSURES/HOUSINGS/SHELTERS

**AMPTEK**  
781-275-2242

## CALIBRATION EQUIPMENT/SERVICES

Ancal  
Applied Image  
Artel  
Bangs Labs

Brookfield AMETEK  
Instrumentation & Specialty Controls  
CONCOA/Controls Corp America  
Dakota Instruments  
Electro Standards Labs  
Fritsch GmbH  
Milling and Sizing  
GrayWolf Sensing Solutions  
Guided Wave  
H & A Scientific  
Irradian Ltd  
Mesa Labs  
MIL-RAM Technology  
Omega Engineering  
Sierra Instruments

## DATA ACQUISITION/HANDLING SYSTEMS, PROCESS

ABB  
Analytical Measurement  
**ABB Analytical Measurement**  
800-858-3847

Aerotech  
Applied Chemometrics  
Biodata Ltd  
Buchi Corp  
getSpec.com  
H & A Scientific  
MKS Instruments  
Omega Engineering  
Pentek  
TAL Technologies

## FIBER OPTICS AND RELATED PRODUCTS

art photonics GmbH  
**Avantes**  
Calmar Laser  
Electro Standards Labs  
FiberTech Optica  
Guided Wave  
H & A Scientific  
InPhotonics  
J&M Analytik AG  
Laser Components USA  
LT Industries  
OZ Optics Ltd  
Piezosystem Jena GmbH  
Schott North America  
Lighting & Imaging  
Terahertz Technologies  
US Fiberoptec Technology

## LABELS AND LABELING EQUIPMENT

Bel-Art - SP Scienceware  
DPSS Lasers

## SAFETY EQUIPMENT

Advanced Specialty Gas Equipment  
CT Intl  
**Electro Optical Products Corp**  
718-456-6000  
ENMET  
HEMCO Corp  
Justrite Mfg Co  
MIL-RAM Technology  
Parker Balston  
Filtration & Separation Div, Parker  
Hannifin Corp  
S E Intl  
Sensor Electronics Corp

## SAMPLE CONDITIONING SYSTEMS, GAS

CONCOA/Controls Corp America  
**Simplex Scientific**  
808-831-4476

## SOFTWARE, CHEMOMETRICS

Applied Chemometrics  
Buchi Corp  
H & A Scientific  
Infometrix  
LT Industries

## SOFTWARE, INSTRUMENT CONTROL

**ABB Analytical Measurement**  
800-858-3847  
**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770

Applied Chemometrics  
Biodata Ltd  
Blue Mountain Quality Resources  
LT Industries  
Pentek  
TAL Technologies  
Windmill Software Ltd

## SOFTWARE, VALIDATION

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770

Applied Chemometrics  
Blue Mountain Quality Resources  
Integrated Engineering Software  
PACS Courses & Conferences,  
Training & Testing

**Thermo Scientific - Molecular Spectroscopy**  
Part of Thermo Fisher Scientific  
800-532-4752

## VALVES, FITTINGS, FLANGES

Aalborg Instruments  
Advanced Specialty Gas Equipment  
Bel-Art - SP Scienceware  
Brooks Instrument  
Clark Solutions  
CONCOA/Controls Corp America  
Dakota Instruments  
Exair Corp  
MKS Instruments  
Parker Balston  
Filtration & Separation Div,  
Parker Hannifin Corp  
Parker Hannifin  
Precision Fluidics  
Peter Paul Electronics Co  
Qosina  
Qosmedix  
Vat  
Vita Needle Co

**BIOANALYZERS AND RELATED EQUIPMENT****AUTOSAMPLERS**

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770

Braintree Scientific  
Fritsch GmbH  
Milling and Sizing  
LEAP Technologies  
LT Industries  
Meadows Instrumentation  
Parker Hannifin  
Precision Fluidics  
Teledyne CETAC Technologies

**BIOSENSORS**

Coates Consulting  
Daylight Solutions  
getSpec.com  
Laser Components USA  
optek-Danulat

**CHROMATOGRAPHY, GAS**

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770

Angstrom-Advanced  
CeramTec North America  
Laurens Operations  
CONCOA/Controls Corp America  
Meadows Instrumentation  
OI Analytical

**Shimadzu Scientific Instruments**  
Email: webmaster@shimadzu.com  
www.ssi.shimadzu.com  
fax 410-381-1222  
800-477-1227

**CHROMATOGRAPHY, ION**

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770

Cecil Instruments Ltd  
CeramTec North America  
Laurens Operations  
Meadows Instrumentation  
The Nest Group

**CHROMATOGRAPHY, LIQUID**

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770

Angstrom-Advanced  
Boston Express Lab  
Campro Scientific GmbH  
Cecil Instruments Ltd  
Chiralizer Services LLC  
**JM Science**  
Meadows Instrumentation  
The Nest Group  
optek-Danulat  
PolyLC

**Shimadzu Scientific Instruments**  
Email: webmaster@shimadzu.com  
www.ssi.shimadzu.com  
fax 410-381-1222  
800-477-1227

SPECTRO Analytical Instruments  
Div of Ametek  
Wyatt Technology Corp

**CHROMATOGRAPHY, OTHER**

Denville Scientific  
Meadows Instrumentation  
Miles Scientific (Analtech)  
The Nest Group

**ELECTROPHORESIS, CAPILLARY**

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770  
Braintree Scientific  
TREK

**ELECTROPHORESIS, GEL**

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770

BioDesign of New York  
Crescent Chemical Co  
Soltec Ventures  
USA Scientific  
UVP LLC

**ELECTROPHORESIS, OTHER**

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770

Crescent Chemical Co  
Inotech Bioscience, LLC  
Soltec Ventures  
UVP LLC  
Wyatt Technology Corp

**FLUORIMETERS**

BioTek Instruments  
BMG LABTECH GmbH  
**Edinburgh Instruments**  
Photonics  
+44-1506-425-300  
**HORIBA Scientific**  
Quantum Northwest  
Turner Designs

**GAMMA COUNTERS**

Boston Express Lab  
Industrial Test Systems

US Nuclear Corp  
Technical Assocs  
XIA LLC

**IMMUNOASSAYS, AUTOMATED**

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
800-227-8770  
BioTek Instruments

**LIQUID CHROMATOGRAPHY-MASS SPECTROMETERS**

**Agilent Technologies**  
Life Sciences & Chemical Analysis  
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Fax: 978-536-2205  
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Fax: 201-748-6088  
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Email: info@z-laser.de  
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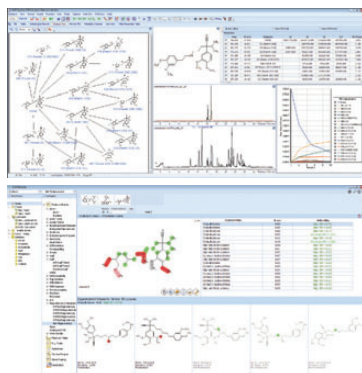
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# PRODUCT PROFILES

## MetaSense—Efficient, Comprehensive Metabolite Identification

Reduce the bottleneck of LC-MS data analysis and facilitate knowledge sharing with software that meets the requirements of scientists that undertake detailed metabolism studies and colleagues that benefit from study results.



- Simplify data analysis with one software interface to natively process and analyze all your LC-MS data (option to automate for greater productivity)
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- Detect and identify expected and unexpected metabolites through the combined approach of metabolite prediction and LC-MS data analysis
- Capture all the relevant spectra and chromatograms, with associated metabolites, in a centralized database for review and interrogation.
- Share assembled, searchable, live analytical and chemical data through web-based visualization tools for faster decision-making.

### Advanced Chemistry Development, Inc. (ACD/Labs)

Ontario, Canada

[www.acdlabs.com/MetaSense](http://www.acdlabs.com/MetaSense)

## Portable Mass Spectrometer

BaySpec Portability is a compact lightweight (<10 kg) mass spectrometer specifically designed for field applications. It uses a miniature linear ion trap mass analyzer, which provides high sensitivity and low detection limits. The instrument is equipped with two independent inlets, one for electron ionization and another for atmospheric pressure ionization. It is compatible with electrospray, thermal-desorption electrospray, APCI, and most of the ambient ionization techniques such as DART and DESI. The Portability is ideal for trace in situ analysis in many demanding applications, such as process control, detection of explosives and warfare agents, or screening for pesticides and other environmental contaminants.

### BaySpec, Inc.

San Jose, CA

[www.bayspec.com](http://www.bayspec.com)



## UV-vis Validation Kit



The IN-SPEC® reference materials are inert and NIST traceable. Kit# 87020 is an easy way to verify your UV-vis spectrophotometer's photometric accuracy, wavelength scale, and stray light. This ready-to-use kit includes both polymeric photometric accuracy standards, Holmium Oxide and Potassium Iodide. The pourable reference materials eliminate the need for sealed cuvettes and provide an economical solution for the laboratory. By using these, one also validates cleaning procedures and quartz cell integrity.

### GFS Chemicals, Inc.

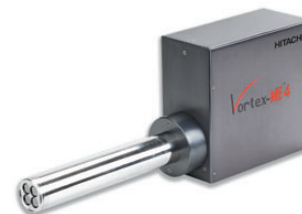
Columbus, OH

[www.gfschemicals.com](http://www.gfschemicals.com)



## Hitachi X-ray Technology

The Vortex® line from Hitachi High-Technologies Science leads the industry in X-ray detection. From demanding synchrotron applications where count-rate is THE metric, to analytical instruments requiring high resolution and a broad range of sensitivity, there is a Vortex® detector to meet just about any need. In fact, Vortex® detectors are found in most synchrotron facilities around the world as well as in our very own line of ED-XRF instruments; both the thin-film measurement and elemental analyzer models. Contact Hitachi today to talk about your X-ray application.



### Hitachi High Technologies America, Inc.

Northridge, CA

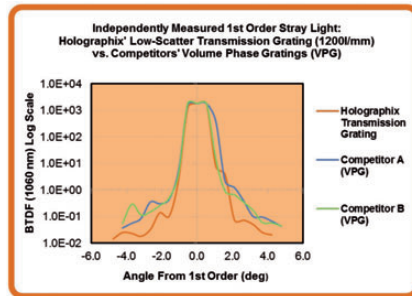
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## Low Stray Light Transmission Gratings

Holographix LLC expands its capabilities in the area of cost-effective replicated transmission gratings with the introduction of our custom designed and manufactured, high efficiency, low stray light transmission gratings. Recent independent testing confirms that Holographix' transmission gratings provide a lower stray light solution compared to volume phase transmission gratings. From design and prototyping, to mass production, we are your custom source for transmission gratings!



### Holographix LLC

Hudson, MA  
www.holographix.com

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## Optical Filters for Spectroscopy and Biophotonics

Iridian's family of optical filters for spectroscopy/biophotonics offer high transmittance with low ripple in emission bands along with deep and steep blocking of excitation sources providing "more signal with less background" to instruments in applications



such as Raman spectroscopy, confocal fluorescence imaging, flow cytometry, and point-of-care clinical analyzers. Iridian specializes in tailoring custom solutions to meet specific optical, physical, and commercial needs of OEM instrumentation customers, and commonly used standard filters are available for purchase online. All of Iridian's filters are manufactured using robust and reliable sputtering processes, ensuring long-term stable performance.

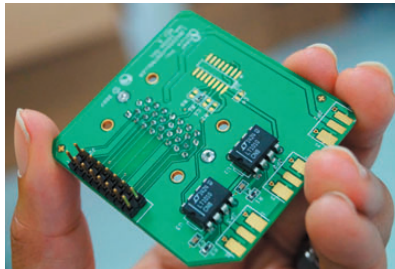
### Iridian Spectral Technologies

Ottawa, Ontario, Canada  
www.iridian.ca



## Popular OEM Spectrometers

Ocean Optics provides a variety of modular optical sensing solutions for diverse applications such as biomedical and life sciences research, food safety and authentication, agricultural monitoring, science education, and quality control. The company has specified and delivered more than 250,000 miniature and modular spectrometers over the past two decades. Ocean Optics provides a comprehensive range of complementary technologies, including software, chemical sensors, Raman instrumentation, optical fibers, probes, filters, and many more spectroscopic peripherals and accessories. Our modular spectrometers and sensors are ideal for integration into instruments. We offer our knowledge and a consultative sales engineering team to support the customization required by OEM customers.



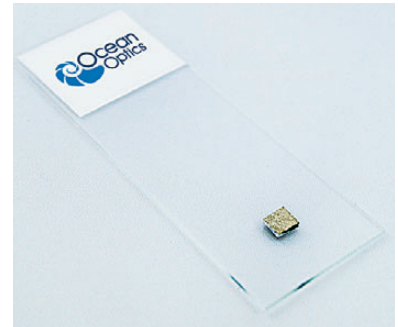
### Ocean Optics

Dunedin, FL  
www.oceanoptics.com



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Our gold, silver, and nanosponge gold/silver SERS substrates let you make fast, repeatable SERS measurements for the identification and quantification of SERS-active analytes. Typical applications include trace level detection of explosives and narcotics and precision screening of food ingredients for controlled additives such as melamine and pesticides. SERS substrates also can be used for authentication and anti-counterfeiting applications using SERS-active taggants. Unlike many existing SERS products on the market, Ocean Optics SERS substrates are easy to use, affordable, and can be mass produced with high repeatability for routine deployment in the laboratory or field.



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# PRODUCT PROFILES

## Low-Frequency Raman Modules

Ondax's upgraded line of **THz-Raman® Spectroscopy Modules** simultaneously measure both chemical composition and molecular structure in a single measurement for any process or laboratory environment.

The **TR-PROBE** and **TR-BENCH** modules share a new versatile, interchangeable sample collection interface, compatible with a wide variety of vial and tablet holders, immersion probe tips and free-space, focused-beam options. This enables flexible solutions for in-situ process monitoring, immersion, bulk or sample testing applications. The **TR-MICRO** is configured to mount to virtually any scientific-grade microscope for high-resolution and mapping applications.

Available in 532 nm, 785 nm, 850 nm, 976 nm and 1064 nm wavelengths.

**Ondax, Inc.**  
Monrovia, CA  
www.ondax.com



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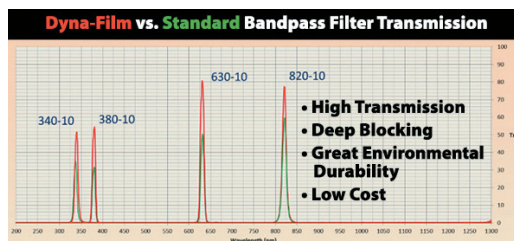
The Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) system delivers comprehensive, instant gas analysis to trace pptv levels. Now available with high-throughput continuous sample analysis, the Voice200ultra from Syft Technologies utilizes direct, ultra-soft chemical ionization. Using eight instantly switchable mass-selected reagent ions enable detection of a very wide range of challenging compounds like ammonia, formaldehyde, hydrogen chloride, and hydrogen sulfide. The system combines extremely high selectivity with push-button simplicity—all without requiring sample preparation. Value-added financing plans, including rent, lease, or zero down and zero interest financing, are available.



**Quantum Analytics**  
Foster City, CA  
www.LQA.com



## Dyna-Film Optical Bandpass Filters



Dyna-Film Optical Bandpass Filters are designed to optimize spectral performance, provide exceptional environmental durability, and minimize the cost of optical bandpass filtering required for absorbance, reflectance, and transmissive applications. Bridging the gap between traditional bandpass filters and expensive budget busting sputtered films, Optometrics has combined best practices learned over the past 40 years as a leading manufacturer of catalog and OEM optical filters, with today's advanced materials, construction methods, and large volume manufacturing capabilities. Dyna-Film Optical Bandpass Filters exhibit the following critical spectral and physical performance characteristics:

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- Deep Blocking
- Great Environmental Durability
- Low Cost

**Optometrics**  
Littleton, MA  
www.Optometrics.com



## Automated Infrared Microscope

Shimadzu's fully automated AIM-9000 allows performing all steps in micro analysis quickly and easily. The system's wide field camera is equipped with a 330x magnification zoom function that provides analysts with an easier and more efficient tool for macro viewing and micro analysis. The system also features automatic contaminant recognition by setting an aperture on measurement spots automatically, a contaminant analysis program for easier identification, and a high-speed mapping program. In addition, it offers the industry's best S/N ratio of 30,000:1, allowing users to quickly obtain excellent spectra from even the smallest contaminants.



**Shimadzu Scientific Instruments**  
Columbia, MD  
www.ssi.shimadzu.com



# PRODUCT PROFILES

## Pyrolyzer for FT-IR

The SupraTherm-PRO Pyrolyzer from Simplex Scientific is designed specifically for use with FT-IR. Pyrolyzing samples at high temperatures is a useful method of material analysis when combined with FT-IR gas analysis. The SupraTherm can sample large volumes of materials at slow heating rates to maximize separation of the evolved gases. It heats to 900 °C, and can be nitrogen purged. The included software provides programmable temperature control and tracking. A complete pyrolysis system with gas cell and transferline is also available.



**Simplex Scientific**  
Middleton, WI  
www.simplexsci.com



## Sample Preparation Press

The hydraulic Atlas Autotouch Press is a hugely popular sample preparation device which not only simplifies pellet-pressing but makes it safer.

This bench-top press has fully programmable, microprocessor-controlled, power-assisted hydraulics for ease-of-use and repeatability.

With a small footprint, ergonomic design and low noise characteristic, the press is appropriate for a range of applications in both modern laboratories and heavy industrial environments.

The press is fully compatible with Specac Pellet Die assemblies and other Specac Sample Preparation accessories, which makes it ideally suited for XRF and FT-IR pelletizing applications in atomic and molecular spectroscopy.



**Specac Inc.**  
Swedesboro, NJ  
www.specac.com

## MicroNIR™ Spectrometers

Offering the highest performance-to-price ratio in the industry, the ultra-compact MicroNIR™ family of spectrometers is solving customer needs across

multiple industries. Measuring wavelengths of 950–1650, the MicroNIR OnSite™ integrates all components into a small hand-held unit suitable for convenient, portable use in the field or on the factory floor. The MicroNIR OnSite is controlled by tablet PC based software with an intuitive user interface. MicroNIR PAT-W™ and PAT-U™ are designed for on-line or at-line process monitoring and control. The battery-powered, rugged MicroNIR PAT spectrometers are equipped with WiFi connectivity for data communication. The MicroNIR enables real-time, non-destructive evaluations anywhere.



**Viavi Solutions**  
Milpitas, CA  
www.viavisolutions.com/micronir

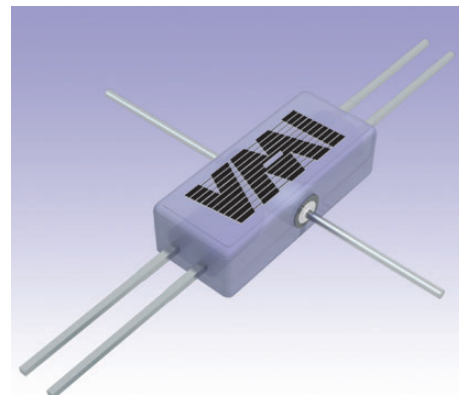
## Optocouplers

Choose from 10 kV, 15 kV, or 50 kV optocouplers used to prevent ground loops in noisy environments where instruments are used. The linear reverse leakage current output, when the optocoupler is reverse-biased, is useful in control circuitry, feedback loops, or when used as a high voltage switch or op amp.

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# Accelerating Trace Metal Analysis



**Anton Paar**



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The Multiwave GO is a compact high-throughput microwave digestion system that can process up to 12 samples in as little as 18 minutes. The Directed Multimode Cavity with Smart-Vent technology eliminates consumables and enables samples to be rapidly heated and cooled.

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