Introduction

PerkinElmer’s hyphenated solutions couple two or more instruments to greatly increase the power of analyses and save precious time by acquiring more information from a single run. PerkinElmer TGA 8000™ and STA systems coupled with FT-IR, MS, and/or GC/MS instruments represent the industry’s most complete and advanced line of hyphenated platforms for materials characterization in polymers, pharmaceuticals, chemicals, petroleum, rubber, and food. Its applications include identifying harmful chemicals in soil, quantitating components in polymers, determining leachables that may contaminate a product’s packaging, and identifying phthalates in PVC samples.

The following pages will give you a basic overview of the most commonly used techniques and provide the information necessary to help you select the one that best suits your specific needs and applications.
What Does Hyphenated Technology Mean?
In short, hyphenated technology simply means connecting two or more instruments together to enhance material characterization. Connecting a TGA to a Mass Spectrometer (TG-MS) is an example of a hyphenated technology. In the plastics industry, for instance, Thermogravimetric Analysis (TGA) coupled with Fourier Transform Infrared Spectroscopy (FT-IR) is a common technique used to study the weight loss and chemical components of the evolved off gas during heating.

Why Is This Important?
Think about plasticizers that are added to polymeric material to increase its flexibility, from those ubiquitous plastic ties to plastic bottles. These plasticizers change many properties of the original polymer and often contain phthalates. Since plasticizers are usually made up of small molecules, they also tend to migrate to the surface and evaporate from the polymer over time or upon heating. Remember that new car smell? More ominous, however, are the apparent health issues associated with plasticizers such as phthalates migrating from some plastic products to humans.

That is where the use of hyphenated technologies such as the PerkinElmer TGA 8000™ and Frontier™ FT-IR system comes in handy to provide scientists and manufacturers with a more complete picture of a polymeric material's characterization. Oftentimes that kind of analysis can lead to better product performance, reduced costs, and improved recyclability. And sometimes, as in the discovery of Bisphenol A (BPA) in plastics and in our foods, hyphenated technologies like those offered by PerkinElmer are helping to save lives, too.

PerkinElmer TGA and STA systems coupled with FT-IR, MS, and/or GC/MS instruments also represent the industry's most complete and advanced line of hyphenated platforms to help better understand how materials degrade, gases evolve, identifying components/contaminates and how materials respond to a nonstandard test environment like high UV levels or humidity changes. Hyphenation with PerkinElmer’s award-inning instrumentation will reveal new information and insights that will provide your laboratory with a competitive advantage that is simply not available to single systems users.

The World Leader in Hyphenated Technology
PerkinElmer has been at the forefront of material characterization analytical technology for over 75 years. We have been offering total solutions for material research and development, from thermal analysis to wide-range molecular spectroscopy till the more advanced hyphenated technology. We can provide the ideal solution no matter what the specifics of your application. We understand the unique and varied needs of the customers and markets we serve. Take it from experience and the only company in the industry capable of making, supporting, and servicing combined systems that streamline and simplify the entire process from sample handling and analysis to the communication of test results. Hyphenation with PerkinElmer will provide your lab with new pathways for innovation and scientific understanding.

Sample Modification in Testing

Techniques where various instruments are coupled together to change the sample while it is being monitored. UV-irradiation of a sample in DSC or hooking a humidity generator to a DMA are both examples of this approach.

Evolved Gas Analysis

Measurement of the gases evolved from a sample being tested by a thermal analyzer such as TGA, STA and GC. These gases can be released from a reaction, by evaporation, boiling, separation, or from the combustion of a material. The most well known is TGA-FT-IR where the IR is used to identify the off gases from a TGA experiment. Another example would be GC-ICP-MS where the GC helps speciate the sample before ICP-MS testing.

Simultaneous Analysis

Use of two or more techniques, like DSC-Raman, DSC-NIR, or DTA-ATR, to measure the same sample at the same time. A simultaneous thermal analyzer (STA) can be considered the simplest form of this technique.

<table>
<thead>
<tr>
<th>Sample Modification in Testing</th>
<th>Evolved Gas Analysis (EGA)</th>
<th>Simultaneous Analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td>UV-DSC</td>
<td>TG-IR</td>
<td>DSC-Raman</td>
</tr>
<tr>
<td>UV-DMA (Controlled Humidity)</td>
<td>TG-MS</td>
<td></td>
</tr>
<tr>
<td>CH-DMA (Controlled Humidity)</td>
<td>TG-GC/MS</td>
<td></td>
</tr>
<tr>
<td></td>
<td>TG-IR-GC/MS</td>
<td></td>
</tr>
<tr>
<td></td>
<td>GC-ICP-MS</td>
<td></td>
</tr>
</tbody>
</table>
## Comparison of Hypernated Technologies

<table>
<thead>
<tr>
<th>System</th>
<th>Configuration</th>
<th>Strengths</th>
<th>Limitations</th>
<th>Applications</th>
</tr>
</thead>
<tbody>
<tr>
<td>TG-IR</td>
<td>Spectrum Two FT-IR – TL8000 – STA 6000/ TGA 4000</td>
<td>• Functional group analysis</td>
<td>• Lower sensitivity</td>
<td>• Industrial – competitive analysis, process optimization</td>
</tr>
<tr>
<td></td>
<td>Frontier FT-IR – TL8000 – STA 6000/TGA 4000</td>
<td>• Vapor phase libraries</td>
<td></td>
<td>• Food – simplifies sample preparation</td>
</tr>
<tr>
<td></td>
<td>Frontier FT-IR – TL8000 – STA 8000</td>
<td>• Allows structural isomers</td>
<td></td>
<td>• Environment – contaminated soil</td>
</tr>
<tr>
<td></td>
<td>Spectrum Two FT-IR – TL8000 – TGA 8000</td>
<td>• Real time analysis</td>
<td></td>
<td>• Pharmaceutical – residual solvent</td>
</tr>
<tr>
<td></td>
<td>Frontier FT-IR – TL8000 – TGA 8000</td>
<td>• Qualitative analysis</td>
<td></td>
<td>• Unknown identification</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Non-destructive on vapor</td>
<td></td>
<td>• Decomposition studies</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Lower cost</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TG-MS</td>
<td>Clarus SQ8 MS – TL8300 – TGA 8000</td>
<td>• Fast analysis times</td>
<td>• Mass range limited (1200 amu)</td>
<td>• Industrial – nanomaterials, polymer additives, process optimization</td>
</tr>
<tr>
<td></td>
<td>Clarus SQ8 MS – TL8300 – STA 6000</td>
<td>• High sensitivity</td>
<td>• Limited library</td>
<td>• Food – study different crops, additives, combustion</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Widely applicable</td>
<td>• More expensive</td>
<td>• Environment – contaminated soil, trace amount</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Real time analysis</td>
<td></td>
<td>• Pharmaceutical – residual solvent</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Quantitative analysis</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TG-GC/MS</td>
<td>Clarus SQ8 GC/MS – TL8500 – TGA 8000</td>
<td>• High sensitivity</td>
<td>• Not real-time analysis</td>
<td>• Industrial – nanomaterials, polymer additives, process optimization</td>
</tr>
<tr>
<td></td>
<td>Clarus SQ8 GC/MS – TL8500 – STA 6000/TGA 4000</td>
<td>• Resolved overlapping events</td>
<td></td>
<td>• Food – study different crops, additives, combustion</td>
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<td></td>
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<td></td>
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<td></td>
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<td></td>
<td>• Improve separation by GC approaches</td>
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<td></td>
<td></td>
<td>• Can use GC library</td>
<td></td>
<td></td>
</tr>
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<td>TG-IR-GC/MS</td>
<td>Frontier FT-IR – Clarus SQ8 GC/MS – TL9000 – TGA 8000</td>
<td>• Functional group analysis</td>
<td>• High initial investment</td>
<td>• Industrial – competitive analysis, nanomaterials, polymer additives, process optimization</td>
</tr>
<tr>
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<td></td>
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<td></td>
<td>• TGA, IR and GCMS can easily be used independently</td>
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<tr>
<td>System</td>
<td>Configuration</td>
<td>Applications</td>
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<tr>
<td>UV-DSC</td>
<td>Photo Accessory – DSC 6000, Photo Accessory-DSC 8000/8500</td>
<td>• Curing Study – curing time and process optimization</td>
<td></td>
<td></td>
</tr>
<tr>
<td>UV-DMA</td>
<td>Photo Accessory – DMA 8000</td>
<td>• Curing Study – curing time and process optimization</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Photo aging study</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH-DMA</td>
<td>Humidity Accessory – DMA 8000</td>
<td>• Modulus changes in various humidity and solvent environment</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DSC-Raman</td>
<td>DSC 8000/8500 – Raman Accessory – Raman</td>
<td>• Pharmaceutical – phase transition and polymorphism study</td>
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<td></td>
<td></td>
<td>• Polymer – phase transition and crystallization behavior</td>
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</tbody>
</table>
The combination of a Thermogravimetric Analyzer (TGA) with an Infrared Spectrometer (TG-IR) is the most common type of Evolved Gas Analysis (EGA) in use today. By heating a sample on the TGA, a sample will release volatile materials or generate combustion components as it burns. These gases are then transferred to the IR cell, where the components can be identified. Because of its ability to detect functional groups, IR analysis allows greater understanding of the processes seen in the TGA.

The PerkinElmer TL8000 transfer line is a state-of-the-art system for TG-IR. Unlike simpler systems that simply move the gas to the TGA, the TL8000 is designed to ensure every component evolved in the TGA is transported to the IR.

Advantages of this System Include:

- Insulated heated transfer line with replaceable SilcoSteel® liner
- Heated zero-gravity-effect ‘ZGCell’ gas cell for the PerkinElmer FT-IR instrument incorporating automatic accessory identification, low volume, and efficient sample area purging
- Control unit incorporating a mass flow controller, particle filters, flow smoothing system, independent transfer line and gas cell temperature controllers, and vacuum pump with exhaust line
- Automatic triggering of IR data collection from the Pyris™ Software
- Spectrum Timebase™ Software for time resolved experiments

This design translates into some distinct advantages giving better data and greater ease-of-use:

- Constant gas flow giving optimum separation between time-resolved peaks
- Reduced mixing of IR signals
- No accumulations of heavy components in the IR cell due to ZGCell design
- Automatically import TGA data in Timebase Software

The TL8000 can be used to connect any of the PerkinElmer TGA/STA instruments to any of our FT-IR’s. This offers you a range of options in terms of price and performance to fit your needs.

The TG-IR system is ideally suited for applications identifying materials evolved on heating, like residual solvents in pharmaceuticals, component identification in the analysis of plastics or rubbers, or the study of the combustion products from burning a sample. An example of the data one can get is shown below from a sample of switchgrass, a material being studied in North America as a possible source of biofuels. As shown in Figure 1, there is a small weight loss at low temperatures and then a much larger one at approximately 250 °C, which corresponds to the burning of the organic matter. This data is imported into the Timebase Software where it can be compared to the total absorbance curve and the area of interest selected for analysis. Here we select 30 minutes in the midst of the burn and look at the spectra of the evolved gases.

Figure 1. The data from the TGA run (top left) is transferred automatically to the Timebase Software and compared to the Gram Schmidt plot (top right). From this data, we can examine regions of interest as shown in the lower center image.
Combining a Thermogravimetric Analyzer (TGA) with a Mass Spectrometer (MS) allows detection of very low levels of impurities. By heating a sample on the TGA, it will release volatile materials or combustion components as it burns. These gases are then transferred to the MS for identification. The sensitivity of TG-MS is a powerful tool for quality control, safety, and product development.

When working with a hyphenated instrument, it is important to understand how each instrument works and how the connection affects them both. PerkinElmer manufactures a wide range of products, from thermal to gas chromatography and from infrared and Raman spectroscopy to Inductively Coupled Plasma (ICP).

Hiden Analytical™ MS Systems:
Hiden Analytical has a reputation for making state-of-the-art mass spectrometers and SIMS. Our collaboration allows us to offer a range of hyphenated solutions that can address diverse laboratory needs.

- 200, 300, and 500 amu systems available
- Mass range is upgradeable post sales
- Operation in Helium
- Variable or Soft ionization to control fragmentation
- Easy to connect transfer line
- In-line filters with wide capillary end
- User friendly software
- Automatic triggering of the MS run at the start of the TGA run

Hiden Analytical systems can be coupled to a range of PerkinElmer products allowing you to configure a system with the type of TGA and MS unit needed to address your particular application and budget needs. PerkinElmer’s TGA systems which can be used with Hiden Analytical Systems are:

- TGA 4000 – our rugged, low cost TGA solution
- STA 6000 – DTA and TGA results simultaneously to 1000 °C
- STA 8000 – DTA and TGA results to 1600 °C

In pharmaceutical manufacturing, small amounts of recrystallization solvents need to be removed before processing the powder. TG-MS allows the detection of low levels of residual solvents as shown below.

In Figure 3, the weight loss in the TGA is very small. Despite that, a clear identification of the material is obtained from the MS. In Figure 4, a blend of solvents coming off in the same temperature range is identified. Shown below, the single weight loss in the TGA is seen to consist of water, ethanol, and acetone.

Figure 2. TGA low-mass platinum microfurnace.

Figure 3. The combined TG-MS is ideal for detecting small traces of residual solvents in pharmaceuticals as shown in the detection of low levels of methylene chloride, above.

Figure 4. The combination of TGA and MS allows one to quantify the weight loss from a material and identify the components being evolved.
PerkinElmer's extensive product range means we can supply a complete system with one party service and support as well as the expertise and knowledge to help you use it effectively.

The PerkinElmer TL8500 transfer line allows you to couple our full range of Thermogravimetric Analyzers (TGA) and Simultaneous Thermal Analyzers (STA) to a PerkinElmer Clarus® SQ 8 GC/MS.

The TG-MS system uses:

- Our range of TGA and STA Systems, to optimize sensitivity to weight loss
- The TL8500 is equipped with a 350 °C transfer line, mass flow control, and pumps. The TL8500 allows connection to other brands of MS
- The Clarus SQ 8, for accurate identification

By using the PerkinElmer Clarus SQ 8 Mass Spectrometer, the same MS used in PerkinElmer’s state of the art GC/MS systems, enjoy the advantages of:

- Operation in helium
- The detection of mass ions up to 1200 daltons
- Soft ionization (adjustable EI) to limit fragmentation of the mass ion
- The ability to add chemical ionization (CI) to decrease fragmentation
- Automatic triggering of the MS run at the start of the TGA run

One of the advantages of TG-MS is it is real time and very sensitive. This has several applications in detecting residual solvents in pharmaceuticals and in measuring additives in polymers. In Figure 5, we see an example of a TGA curve, overlaid with the mass ion peaks for three common solvents.

Another example is the decomposition of rubber in the TGA while the evolved gases are tracked as a function of time (Figure 6).

**Figure 5.** The combination of TGA and MS allow one to quantify the weight loss from a material and identify the components being evolved.

**Figure 6.** When burning a complex material like rubber, the TGA data is often confusing. MS on the evolved gas allows us to determine what comes off in the initial weight loss.
Although TG-MS allows real-time monitoring, it can be confusing due to overlapping events and higher mass ions obscuring those of lower mass. By adding gas chromatography (GC) to the system, these events can be cleanly separated and very low levels of impurities detected.

Heating a sample using the TGA causes a sample to release volatile materials or generate combustion components as it burns. These gases are then transferred to the GC, where the components can be collected on a trapping media, in a gas sampling loop, or deposited on the head of a column. The sample can then be run by GC to separate the material, and the peaks identified by the MS. Because of its ability to detect very low levels of material in complex mixtures, the TG-GC/MS is a powerful tool for quality control, safety, and product development.

• Any of the TGA 4000, STA 6000, STA 8000 or TGA 8000 can be connected depending on degree of precision and temperature range needed.
• The TL8500 transfer line runs at 350 °C and uses pumps and mass flow controllers to deliver a precise flow of gas to the GC/MS. Two sample collection loops are included.
• Clarus SQ 8 GC/MS provides maximum detection of low levels of contaminants.

When working with a hyphenated instrument, it is important not only to understand how each of the instruments work, but also how the connection affects them both. Unlike many instrument companies, PerkinElmer makes a range of products, from thermal to gas chromatography and from Infrared and Mass Spectroscopy to ICP. Because of this experience, PerkinElmer is the only company capable of making, supporting, and servicing a combined TG-GC/MS system.

Coupling the PerkinElmer TGA 8000 to the Clarus SQ 8 GC/MS allows several options to collect the evolved gases. Of these, the use of the chilled oven with the Swafertm to collect the volatiles on the top of the GC column has been found to be most convenient.

A small quantity of dried and ground switchgrass was placed on the TGA pan and weighed using the Pyris software. A rapid TGA analysis based on heating the sample from 30 °C to 1000 °C at 100 °C/min in a nitrogen atmosphere was performed to determine which regions of the weight loss curve were to be further studied using the TG-GC/MS technique.
Hyphenating TG-IR-GC/MS is a powerful approach for analysis of an unknown mixture to determine its primary components and identify additives or contaminants. This information may be needed, for example, to evaluate a competitor’s product or to determine compliance with regulations.

The PerkinElmer TL9000 transfer line is used to allow TG-IR-GC/MS analysis on a sample by moving the off gases to the FT-IR and GC/MS after their evolution in the TGA. It acts as the interface between a TGA or STA, an FT-IR like the Frontier or Spectrum Two FT-IR, and a Mass Spectrometer or GC/MS, such as the Clarus SQ 8.

During the TGA thermal separation of a pigmented aqueous sample, the gases released by the sample were sent to the FT-IR for spectral analysis. The TG-IR data consists of a sequence of spectra, acquired at intervals of around 8 seconds. The standard presentation of the data is the adsorption versus wave number, and this spectral profile of the gases released by the sample is generated for each at roughly a two-degree interval. The TG-IR Spectrum Time Base Software provides a 3D graphical representation, consisting of stacked IR spectra, a feature that provides a snapshot of the entire TG-IR separation.

The TL9000 interface was used to perform a subsequent analysis to confirm the identity of the unknown substance in the aqueous sample. At the time of maximum concentration absorbance of the substance being analyzed, the gas in the IR gas cell was sent to a GC/MS.

Advantages

- TG-IR-GC/MS allows one to gain the advantages of two EGA techniques and compensate for their disadvantages.
- Unlike TGA-GC/MS, the TG-IR-GC/MS retains the relationship between temperature a gas is released at and its components by FT-IR.
- The sequentially measuring of the offgases components by GC/MS allow detection of trace levels too low to be seen in the FT-IR.
Consumables and Accessories

With instruments that are the industry standard worldwide, PerkinElmer accessories, consumables, methods and application support meet the most demanding requirements and are the preferred choice in thousands of laboratories globally.

From the measurement of DNA purity to characterization of the most advanced engineered materials, we provide the widest range of solutions available from one company. FT-IR, FT-NIR, TGA, STA, GC — we have solutions for every lab and every budget.

Our expertise in these technology means you can rely on us. Do you need a simple accessory that provides results with a push of a button, or a high-end lamp with unparalleled sensitivity? What about flexible sample sizes and reduced sample setup time? Higher lab productivity? No problem. Whatever challenge you face in material characterization, we can help you solve it. After all, we created the first commercial IR and FT-IR systems over 60 years ago. Since then, we have continually pioneered the technologies, consumables and supplies to help you learn more about the performance and structure of the materials you analyze at the molecular level.

Define your challenge, and we will help you meet it.

**Experience Better and Reproducible Results with the State-of-the-art Interface.**

All interfaces can be connected between various FT-IR, GC/MS, TGA and STA from any analytical brands to grant you a broad range of options in terms of price and performance to fit your needs.

**Transfer Line Models TL8000, TL8500 and TL9000 Advantages:**

- Highest temperature up to 360 °C to avoid condensation and deposition of evolved gases
- Self supported TL for more reliable results
- Replaceable internally treated liner for an easy maintenance

**Zero-Gravity Cell (ZG-Cell):**

Design allows heavy molecular weight components elimination, providing the cell with little maintenance and more sensitive and accurate data. ZG-Cell is provided with an automatic accessory identification, low volume and efficient sample area purging.

**Mass Flow Controller:**

The interfaces controls the flow instead of the pressure. In analytical terms, this means quantitative results for the detection as well as reproducible analysis without stagnation of corrosive gas in the TGA furnace.
Over 25 Years of Expertise

Your lab produces massive amounts of digital data that you need to sift through, analyze, visualize, and share. The productivity of your lab depends on the integration and automation of processes combined with efficient workflow management.

We bring over 25 years of expertise to the marketplace, having developed innovative technologies that have shaped the informatics landscape such as pioneering chemical drawing software, electronic laboratory notebooks, LIMS and instrument integration applications.

Ensemble for R&D

Supports a wide range of workflows, including free-form, chemistry, formulation, biology screening, bioanalytical, and research LIMS. E-Notebook allows organizations to share data, maintain security and efficient archiving, and provides a full audit trail and 21 CFR 11 compliance. Users easily enter content from Word®, Excel®, PowerPoint®, Acrobat® PDF, ChemDraw and structured data in lists and tables.

Ensemble for QA/QC

Fully meets the needs and requirements of laboratories doing routine testing. iLAB™ LES eliminates paper, automates, controls, and documents test execution and ensures adherence to laboratory procedures. LimsLink™ reduces errors and costs by automating data transfer between instruments, instrument data systems and informatics systems.

ChemDraw®

The chemical drawing industry leader includes stereochemistry recognition and display, ChemNMR with spectral prediction and display, and Name=Struct to interconvert structures and IUPAC names. Now also available on iPad®.

TIBCO Spotfire® Analytics Platform

Empowers scientists to explore their data freely: to visualize instantly, mashup, interact with, and share data at any level of detail. The software helps users answer pressing questions, uncover answers to questions they didn’t know they had, and anticipate what happens next, without requiring special queries from IT.

Protect Your Instruments with PerkinElmer OneSource® Laboratory Services

Now that you’ve made an investment in new instrumentation for your lab, it’s time to protect it. OneSource Laboratory Services can help with routine maintenance and repair service from our team of certified engineers along with expert solutions and carefully engineered programs designed to achieve your best targeted business outcomes.

With over 15 years’ of experience and a proven track record of success, OneSource has a deep knowledge and understanding of laboratory and R&D needs and offers a one-of-a-kind systems approach to success. Through insight and expertise OneSource consultants can pinpoint specific issues that impact efficiencies across all facets of operations, and provide innovative, holistic solutions to address them.

The OneSource team of experts partner with your business looking at the whole picture and from every angle to engineer the right outcome to solve your business challenges and to meet your business goals through the following areas.

- Instrument Service and Repair
- Relocation
- Compliance and Validation
- Laboratory IT Services
- Asset Data Visualization Tools
- Laboratory Efficiency Consulting
- Scientific Staffing Solutions
Markem-Imaje Corp. is a worldwide leader of product identification equipment, software, supplies and services for marking and coding. Markem-Imaje has a very active and busy material characterization laboratory, managed and run to conduct new product research and solve day-to-day product problems.

“Whether I am searching for a new technique or in need of enhancing a current instrument to serve my industry better, PerkinElmer’s willingness to engage our needs enforces our belief that they are the business partner of choice in material characterization. I would like to thank your entire team for being that business partner that is helping me succeed in helping my company succeed.”

– Customer Testimonial from Samuel Apkarian, Markem-Imaje Corp.

For more information, visit http://www.perkinelmer.com/category/hyphenated-technology