



ThermoFisher
S C I E N T I F I C

**Our latest developments in FTIR, NIR and Raman
Spectroscopy - Sofia 20 October 2016**

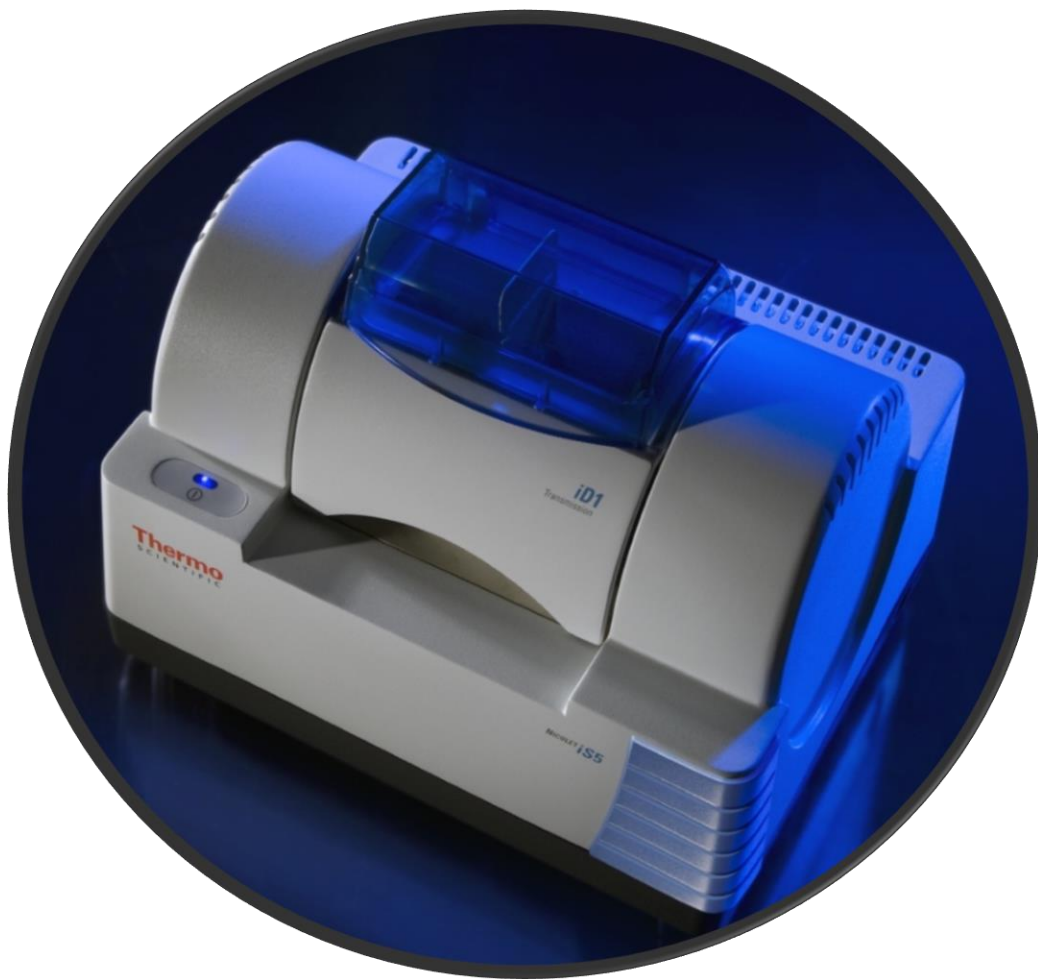
Steve Reynolds
Molecular Spectroscopy Sales Manager

Material and Structural Analysis

- Molecular spectroscopy
 - FT-IR spectrometers, software and accessories
 - FT-IR microscopy and imaging, software, accessories and consumables
 - FT-NIR analysers, software, accessories and consumables
 - Infrared gas analysers
 - Raman spectrometers, software and accessories
 - Vis and UV/Vis spectrophotometers, software, accessories
 - Micro UV
 - NMR



Nicolet iS5 FT-IR Spectrometer



- Premium Performance
- Configurable Sampling Options
- Compact, Rugged Design
- Competitively priced

Nicolet iS10 FT-IR Spectrometer

- 0.4 cm⁻¹ resolution standard
- Signal/Noise 35,000:1
- DTGS standard, MCT-A optional
- External IR beam port
 - Microscope, AEM
- Mid/Near-IR range fixed B/S (KB)
 - Extended range XT-KBr option
- OMNIC Software Integrates:
 - Atmospheric suppression
 - QCheck™ QA/QC Verify Function
 - System Performance Verification
- TGA capabilities



Nicolet iS50 FT-IR Spectrometer

- Multirange data collection
 - Manual or Automatic
- Multiple Sampling Locations
- Multiple Hyphenation Techniques



- Integrated FT-IR Microscope
- Wizard driven data collection and analysis
 - Particles, Laminates, Random mixtures
- Full performance validation
- Transmission, reflection and ATR sampling modes
- High optical efficiency allows room temperature DTGS detector
- MCT-A LN₂ cooled detector option adds superb sensitivity
- Simultaneous viewing, collection and searching



Nicolet Continuum™



- Infinity-corrected optical design
- Single-point microscopy with fast mapping stage
- Dual remote aperture – ultimate spatial resolution
- Dual detector option
- Simultaneous view & collect
- DIC, polarization, fluorescence for visualization
- Transmission, reflection, ATR, Grazing Angle objectives
 - Ge Tip ATR™
- Powerful data processing and visualization software
- USB Digital Camera with software autofocus

DXR Raman Microscope



- Dispersive Raman micro sampling
- Class I Laser-Safe enclosure
- True Confocal microscope design
 - Excellent Depth Profiling
- Spatial Resolution ≤ 1 micron
- Patented Autoalignment
- Integrated components
 - Filters, gratings, lasers
- Patent-Pending autoexposure and autofocus capabilities
- True “Point and Shoot” Raman spectroscopy

DXRxi Raman Imaging Microscope

A total imaging system: hardware and software integration combines **powerful performance** with **image-centric** analysis and **ease of use**



A completely new approach to Raman imaging!

Antaris II™ NIR_{FT-NIR}



- Rugged, reliable FT-NIR analyzer
- Easy to use dedicated analysis RESULT software
- Comprehensive validation and qualification package
- Direct software connection to chemometrics: TQ Analyst™
- OPC: Makes decisions and takes action
- USB control
- Simultaneous transmission and reflection from tablets

Antaris FT-NIR Analyzer Tools



Antaris EX
Explosion Proof

Antaris MX
Multiplexer



Antaris IGS

- Dedicated FT-IR gas analyzer
- Industrial table top & rack mount system configurations
- 0.5 cm⁻¹ resolution at 2 Hz data collect
- Nicolet Series high quality system components: source, laser, interferometer
- RESULT, TQ and ValPro validation
- Integrated heater control and pressure monitoring
- Custom Solutions Services and factory gas calibrations



Introducing the new Nicolet iS5N FT-NIR Spectrometer

- What is the Nicolet iS5N?
 - Extension of the successful iS5 product into the NIR spectral range
 - New entry into the Thermo Scientific NIR portfolio
- Who is the Nicolet iS5N customer?
 - Existing customers looking to deploy routine NIR QC methods
 - Chemical market with incoming and in-process liquid monitoring needs
- NIR Application Opportunities



Nicolet iS5N FT-NIR Spectrometer

Near-infrared for today's laboratory

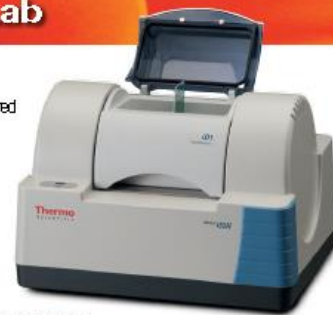
The Nicolet iS5N FT-NIR spectrometer system brings the power of near-infrared to analytical laboratories with minimum hassle and maximum confidence. Method development is made simple by the popular and powerful OMNIC software suite; a familiar environment to thousands of chemists across the globe. Built on the same rugged platform as the iS5, the Nicolet iS5N provides FT-NIR capability in a compact, rugged, cost-effective package designed to meet the needs of today's quality assurance laboratory.

- Extends Nicolet iS5 into NIR range
- Initial Target Market/Customers:
 - Routine NIR liquid analysis
 - Hydroxyl Value, Biodiesel, etc
 - Existing FT-IR customers
 - Chemical industry with routine process monitoring needs

Near-Infrared for Today's Lab

The Nicolet iS5N FT-NIR spectrometer

The Nicolet iS5N FT-NIR spectrometer system brings the power of near-infrared to analytical laboratories with minimum hassle and maximum confidence. Method development is made simple by the popular and powerful OMNIC software suite, a familiar environment to thousands of chemists across the globe. Built on the same rugged platform as the iS5, the Nicolet iS5N provides FT-NIR capability in a compact, cost-effective package designed to meet the needs of today's quality assurance laboratory.



Sampling Flexibility

The large, open sample compartment of the Nicolet iS5N is designed to accommodate a wide range of samples and sampling accessories. The IDH Heated Transmission accessory is a perfect fit, providing temperature control of vials and cuvettes for precise quantitative analysis. The Nicolet iS5N sample compartment is also designed to accommodate any third-party accessories, enabling analysis of a broad range of samples.



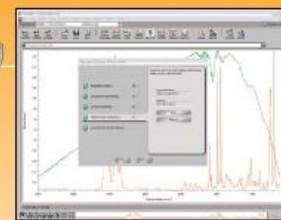
Software that Simplifies Analysis

The Nicolet iS5N is empowered by the popular OMNIC software suite. Quantitative methods can be built simply using Thermo Scientific™ TO Analyst and workflows developed in Thermo Scientific™ OMNIC™ Macros/Basic™. These tools are fully integrated in the OMNIC software suite, making method development and deployment straightforward.



COMPLETE SAMPLING ASSURANCE

System Performance Verification (SPV) monitors and provides status indications for Nicolet iS5 spectrometer models. On-board diagnostics and built-in performance tests ensure the system is working properly. Automatic accessory recognition guarantees consistent analysis conditions, so you get the best possible data. System suitability tests with user-defined QC samples verify method performance, giving you confidence in your results.



System Performance Verification

Nicolet iS5N: Near-IR that fits your lab

Method Development lab

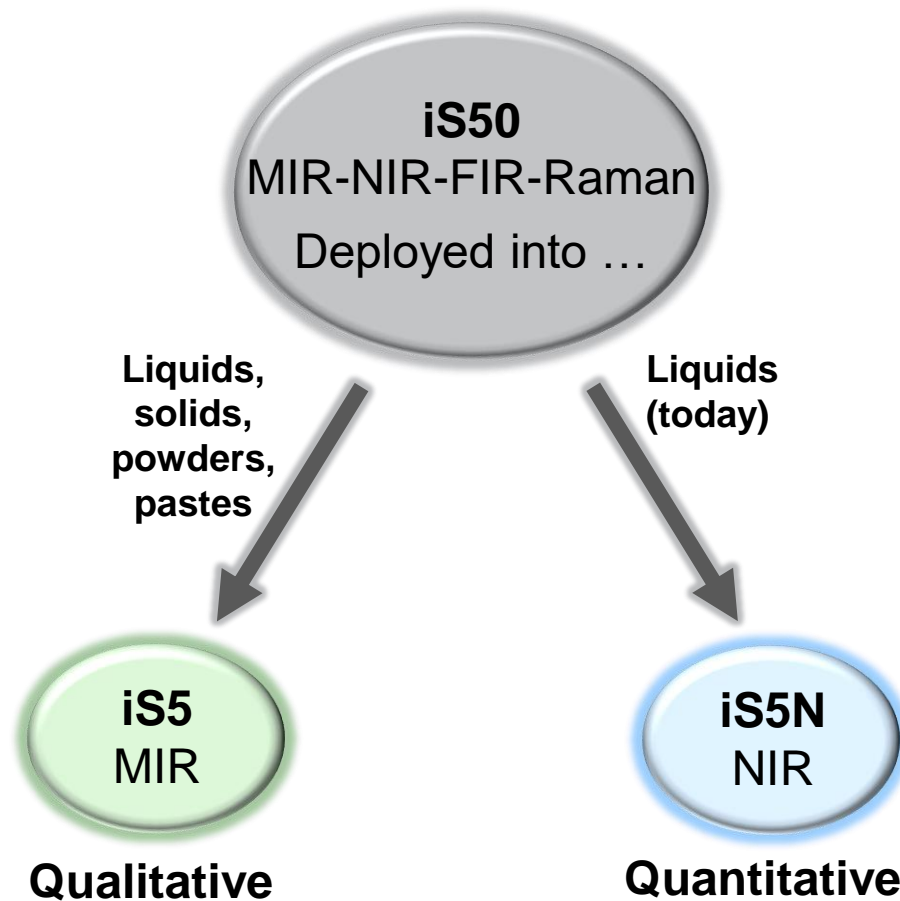


Fiona Fixer – troubleshoots problems, introduces new methods & processes that reduce cost or improve quality & safety

... raw materials, in-process, final QA/QC analysis

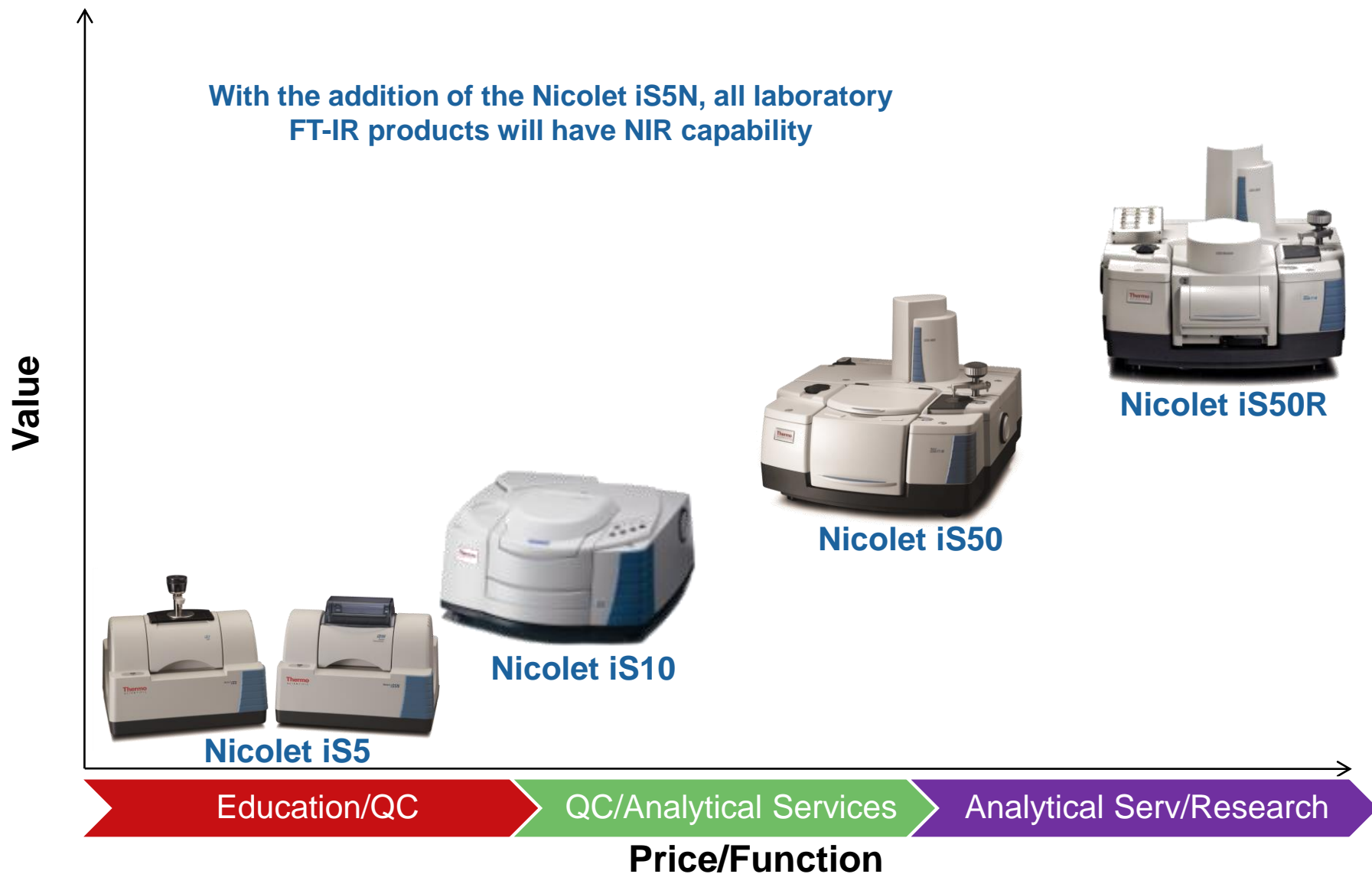


Pam Procedure – ensures product quality and keeps products shipping



OMNIC software familiarity makes it easy for method development labs to deploy iS5N into QA/QC labs

Laboratory FT-IR Current Products



Product Differentiation – Nicolet iS5N vs. Antaris II



Product Attribute	Nicolet iS5N	Antaris II
Target Market	Industrial	Pharmaceutical
Validation Tools	Basic Performance Verification	Full cGMP
Sampling Configuration	Liquid Transmission (at launch)	Dedicated Diffuse Reflection
Lab-to-Line Migration	No	Yes
Software Platform	OMNIC	RESULT
Price point	Similar to Nicolet iS5	Similar to Nicolet iS50

Nicolet iS5N Dedicated FT-NIR Configuration

- **Electrical/Optical**

- Spectral range: 11,000 – 3,800 cm^{-1}
 - Beamplitter: Calcium Fluoride (CaF_2)
 - Detector: Extended range Indium Gallium Arsenide (InGaAs)
 - Source: High intensity halogen
 - User replaceable from bottom plate
 - Laser: Solid state NIR diode, temperature-stabilized
 - Sample compartment windows: Quartz



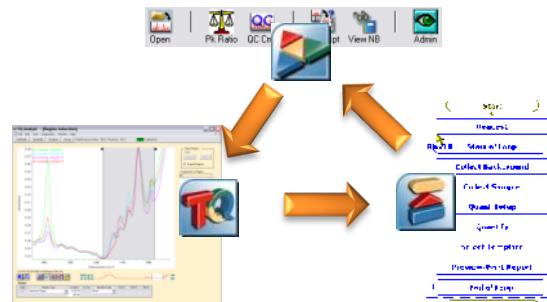
- **Sampling**

- iD1 Transmission accessory (included)
- iD1H Heated Transmission accessory
- Third-party accessories that fit in the iS5



- **Software**

- OMNIC Lite for Nicolet iS5N
- Macros\Basic
- TQ Analyst – EZ or Professional



Introducing the Nicolet iS5N FT-NIR Spectrometer

Obtain fast, accurate testing results with the compact, cost-effective Nicolet iS5N FT-NIR spectrometer. Ideal for Lab & QC managers in the chemical and polymer industries that need to ensure product quality.

- **Marcom Materials**

- Updated Nicolet iS5 brochure, includes iS5N (BR51983)
- Specification sheet (PS52796)
- iD1H Transmission Accessory flyer (FL52807)
- Application Notes:
 - Hydroxyl Value (AN52808)
 - Biodiesel (AN52804)
- Product web page: www.thermoscientific.com/iS5N
- E-mail promotion to:
 - Customer installed base
 - CRM list for general awareness

“Near infrared that fits your QC lab - and your budget”

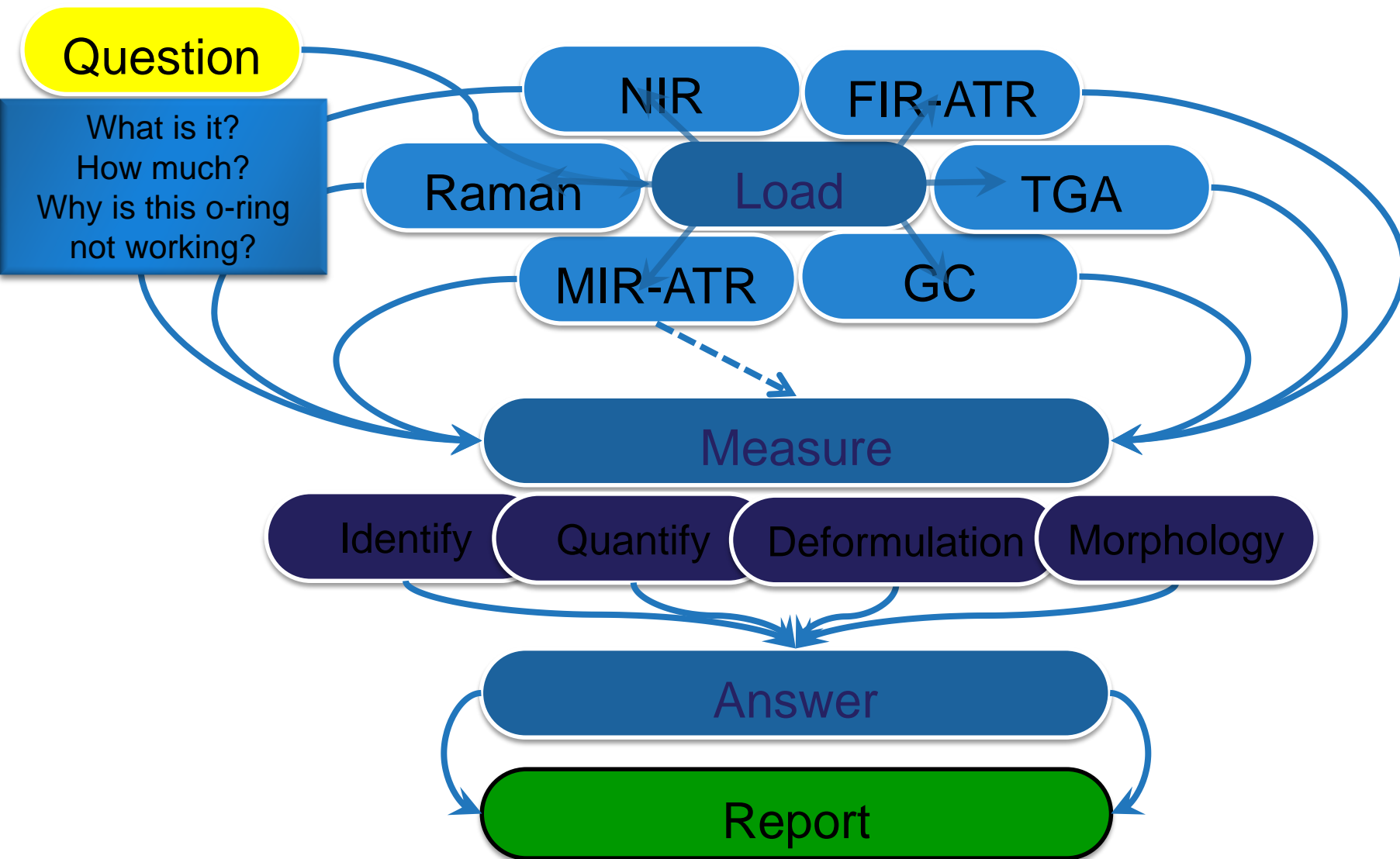


A Nicolet iS50 FT-IR spectrometer is shown in a three-quarter view, positioned over a glowing Earth. The instrument is white with blue accents and features a sample compartment, a detector, and various control knobs and buttons. Labels on the device include 'iS50 ARX' and 'iS50 FT-IR'. The background consists of a dark blue space with several glowing, textured spheres of varying sizes, creating a futuristic and scientific atmosphere.

Nicolet iS50: Unleashing Analytical Power

ThermoFisher
SCIENTIFIC

The Analytical Laboratory Workflow



Discover the Nicolet iS50...

- Unsurpassed **Flexibility**
- Unprecedented **Integration**
- Ultimate **Simplicity**

...Beyond FT-IR, beyond the ordinary, beyond expectations



- Multirange data collection
 - Manual or Automatic
- Multiple Sampling Locations
- Multiple Hyphenation Techniques



Multirange made Simple

- Automatic Beamsplitter Exchange
- Triple Detector Mount
- Total Multi-range control



Flexibility

- Full size sample compartment
- All Smart Accessories supported
- All standard accessories supported

Nicolet iS50

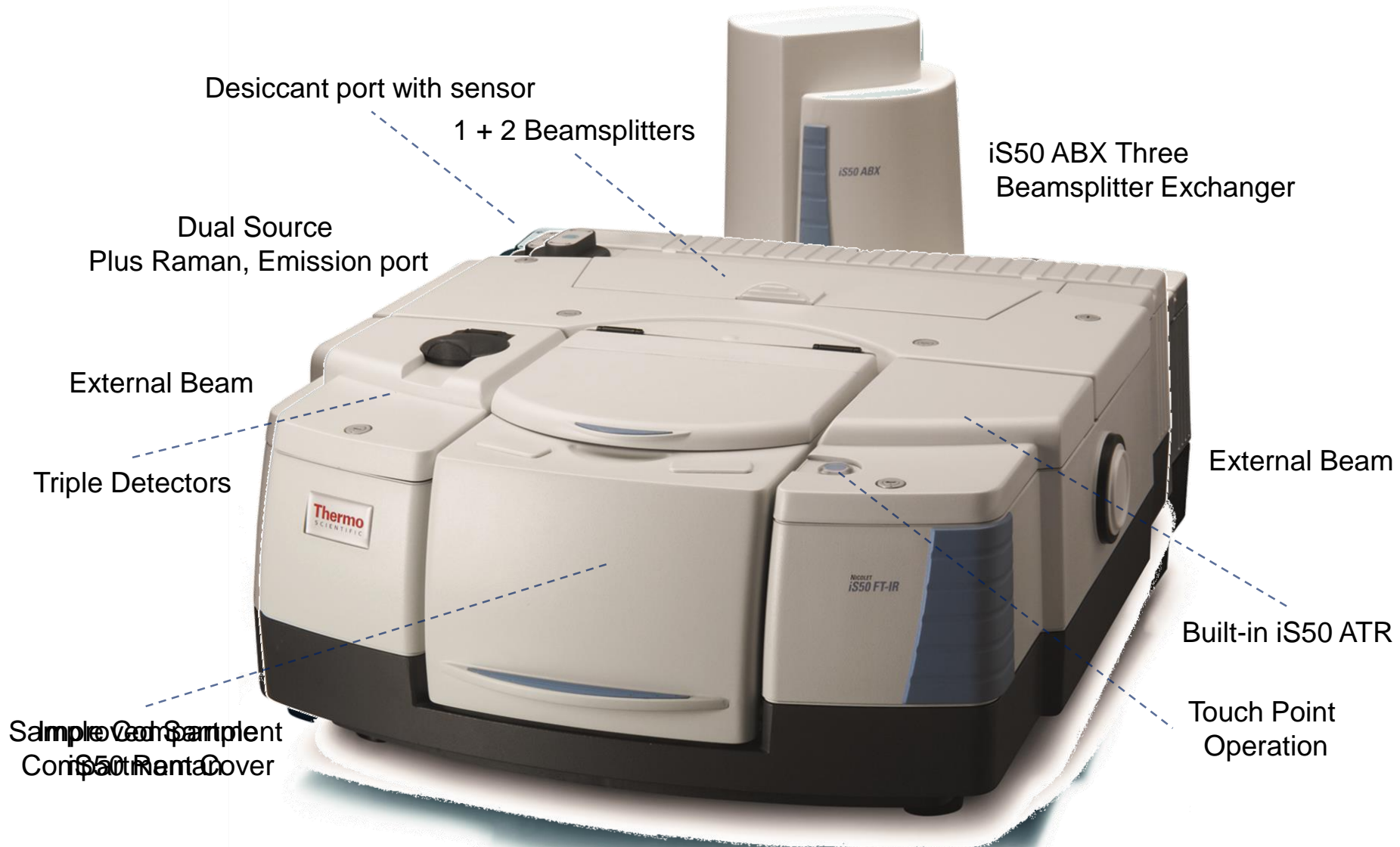


Increased Value

- Smaller Footprint means more laboratory space for other tools
- Great Performance means getting data when the going gets rough
- More Capabilities means have the tools – when you need them

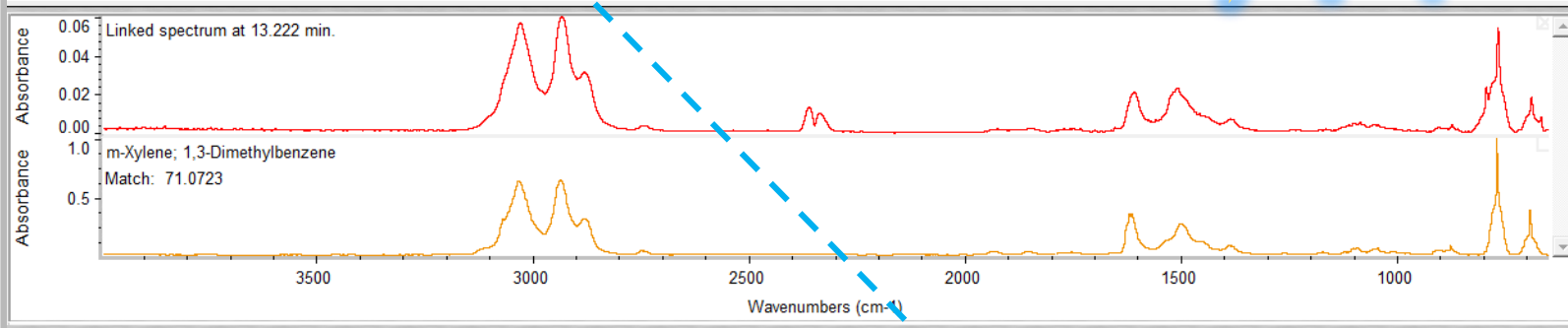
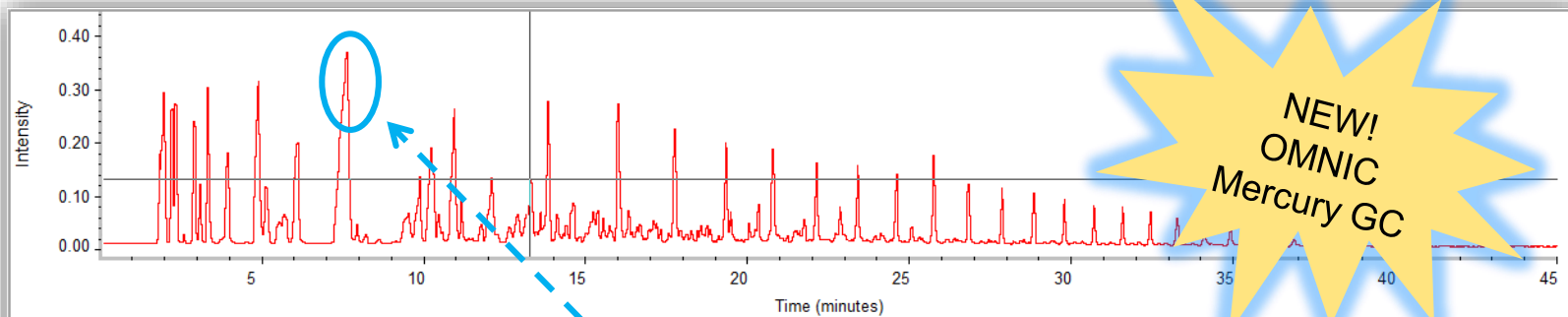
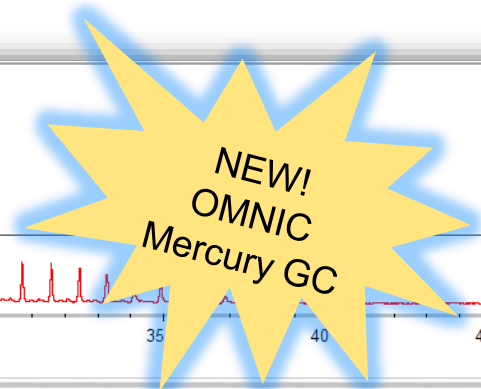


The Nicolet iS50 FT-IR Grows

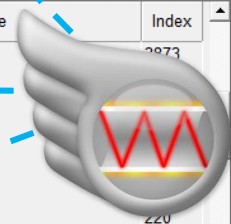


- Continuum FT-IR microscope
- In-compartment TGA-IR
- External GC-IR interface



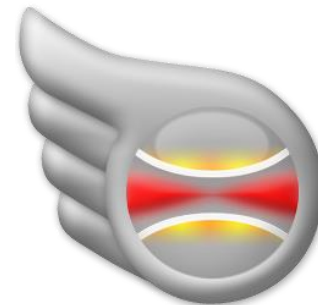


Retention Time	Match	Compound Name	Library Name	Index
8.1250	52.0531	Carbon dioxide	HR Nicolet Vapor Phase	2973
9.4314	78.1214	2-Methylheptane	HR Nicolet Vapor Phase	
9.7819	87.1418	Toluene; Methylbenzene	HR Nicolet Vapor Phase	
10.1324	89.0256	1,3-Dimethylcyclohexane, cis-	HR Nicolet Vapor Phase	
10.3873	60.1657	1,1-Dimethylcyclohexane	HR Nicolet Vapor Phase	
10.8652	93.2497	2-Aminooctane; 1-Methylheptylamine	HR Nicolet Vapor Phase	
11.0883	74.3754	1,3-Dimethylcyclohexane, trans-	HR Nicolet Vapor Phase	
11.6937	70.6362	Mineral spirits; Liqroin	HR Nicolet Vapor Phase	
12.0123	94.0005	Propylcyclohexane	HR Nicolet Vapor Phase	220
12.5540	55.2237	Guaiene; 1,4-Dimethyl-7-isopropylidene-1,2,3,4,5,6,7-	HR Nicolet Vapor Phase	343
12.8089	80.9681	2-Methyloctane	HR Nicolet Vapor Phase	45
13.2231	71.0723	m-Xylene; 1,3-Dimethylbenzene	HR Nicolet Vapor Phase	4421
13.5417	77.5364	2,6-Dimethylcyclohexanemethanol	HR Nicolet Vapor Phase	1005
13.7648	92.1922	Nonane	HR Nicolet Vapor Phase	10
14.0197	76.1310	2-Aminooctane; 1-Methylheptylamine	HR Nicolet Vapor Phase	1705
14.3383	66.4692	Butylcyclopentane	HR Nicolet Vapor Phase	217



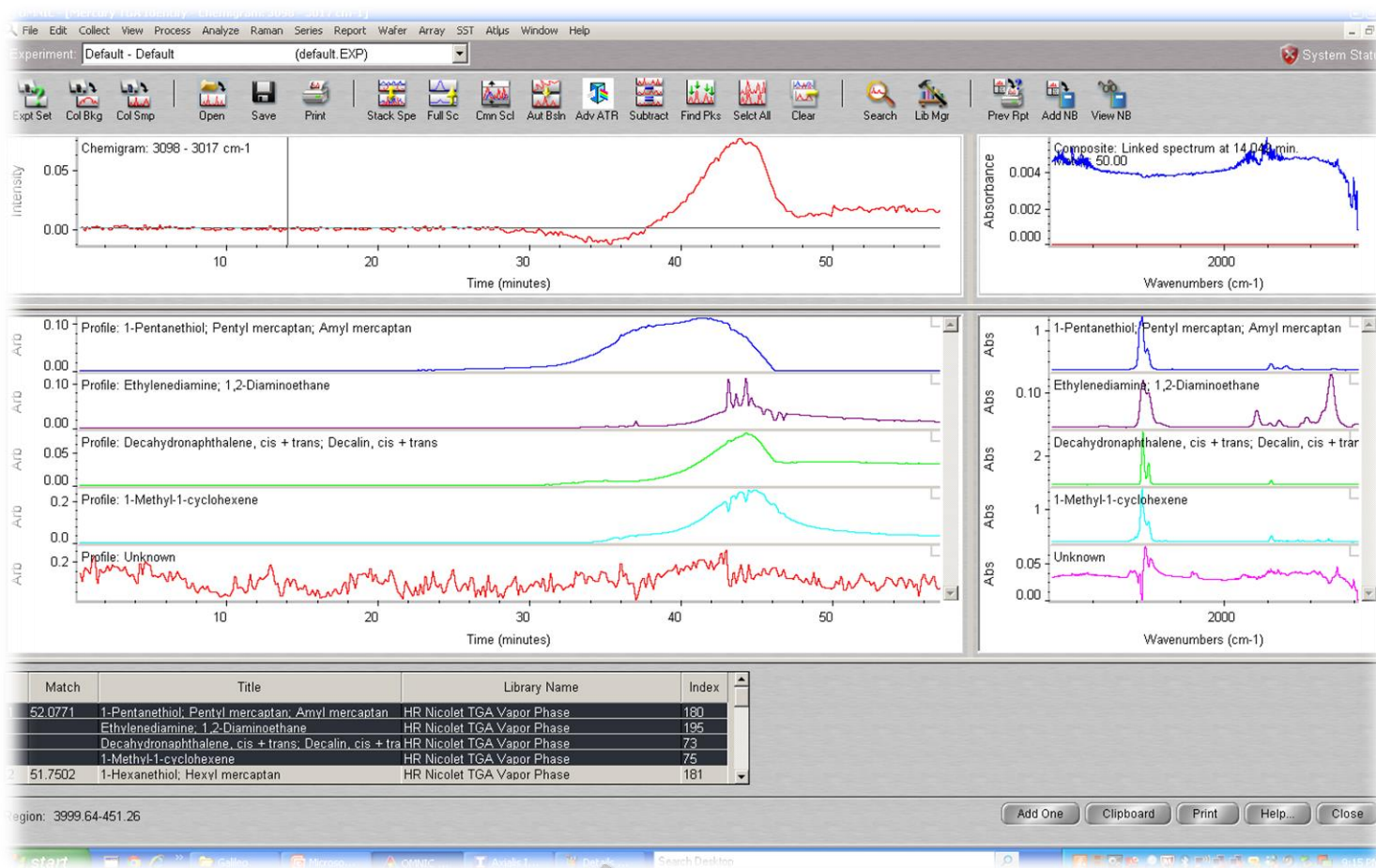
1. Co-adds spectra
2. List peaks by retention time
3. Identifies separated substances

- Same in-compartment interface, now empowered by built-in ATR
 - Smaller foot print and less work
- New OMNIC Mercury TGA software
 - TGA / FT-IR made easy!



NEW!
OMNIC
Mercury TGA





1. Identifies gas species
2. Creates profiles
3. Summarizes material composition

- Up to 5 sampling stations and 3 spectral ranges
- No need to configure optics, or manual set-up
- Touch-Points to “get there” and run samples





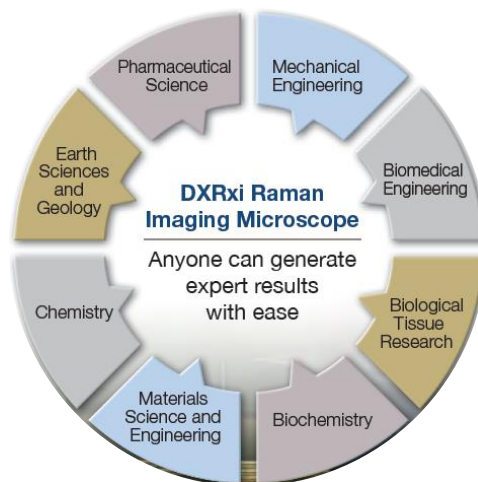
Rethinking Raman Imaging

ThermoFisher
SCIENTIFIC

- The new
- DXRxi Raman Imaging Microscope

The Raman Imaging Value Proposition

The instrument should provide a tool for all users, from basic to advanced

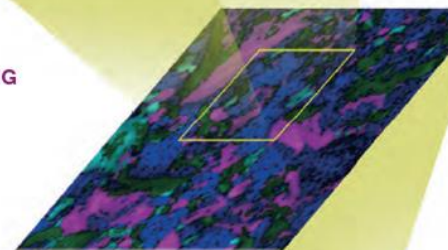


Advanced materials analysis benefits from an image-driven approach

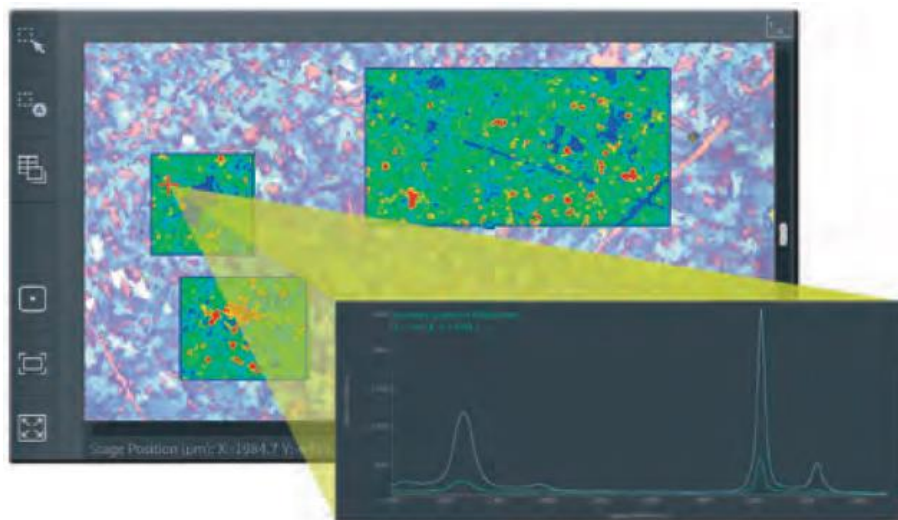
The performance advantage of **FINE DETAIL**



The agility of **RAPID IMAGING**



The **POWER** to look over large areas



Emphasis on microscopy, powered by spectroscopy keeps the answer in focus

The Multiuser Laboratory Toolkit

- **Multiple techniques** are increasingly used with the same sample
- Strong emphasis on **image data** and **data visualization**
- ~70% of those polled use **SEM/TEM**, ~50% use **AFM**
- Work continues to become more **interdisciplinary**, requiring broad **proficiency with many different instruments**



Introducing the DXRxi Raman Imaging Microscope

A total imaging system: hardware and software integration combines **powerful performance** with **image-centric** analysis and **ease of use**



A completely new approach to Raman imaging!

Powerful Integration: “Microscopy First Approach”

“Spectroscopy first”
approach



VS.

“Microscopy first”
approach



OTHER RAMAN INSTRUMENTS

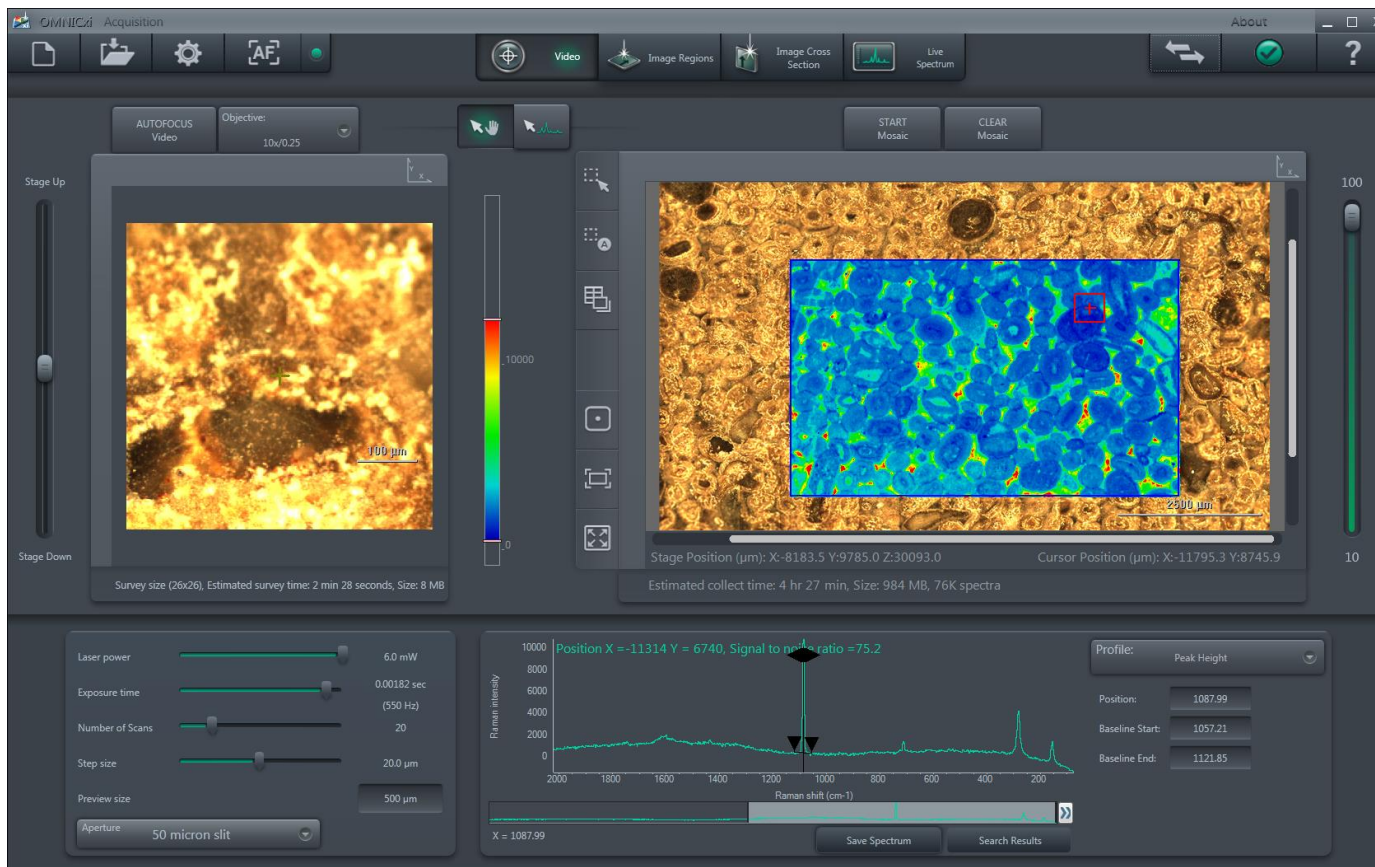
**DXRxi RAMAN IMAGING
MICROSCOPE**

Would you rather be a rat in a maze or an eagle in the sky?

Image Centric Software: OMNICxi for Raman Imaging

Chemical image preview provides one click Raman imaging and instant gratification

Location of video and chemical image previews tied to mosaic

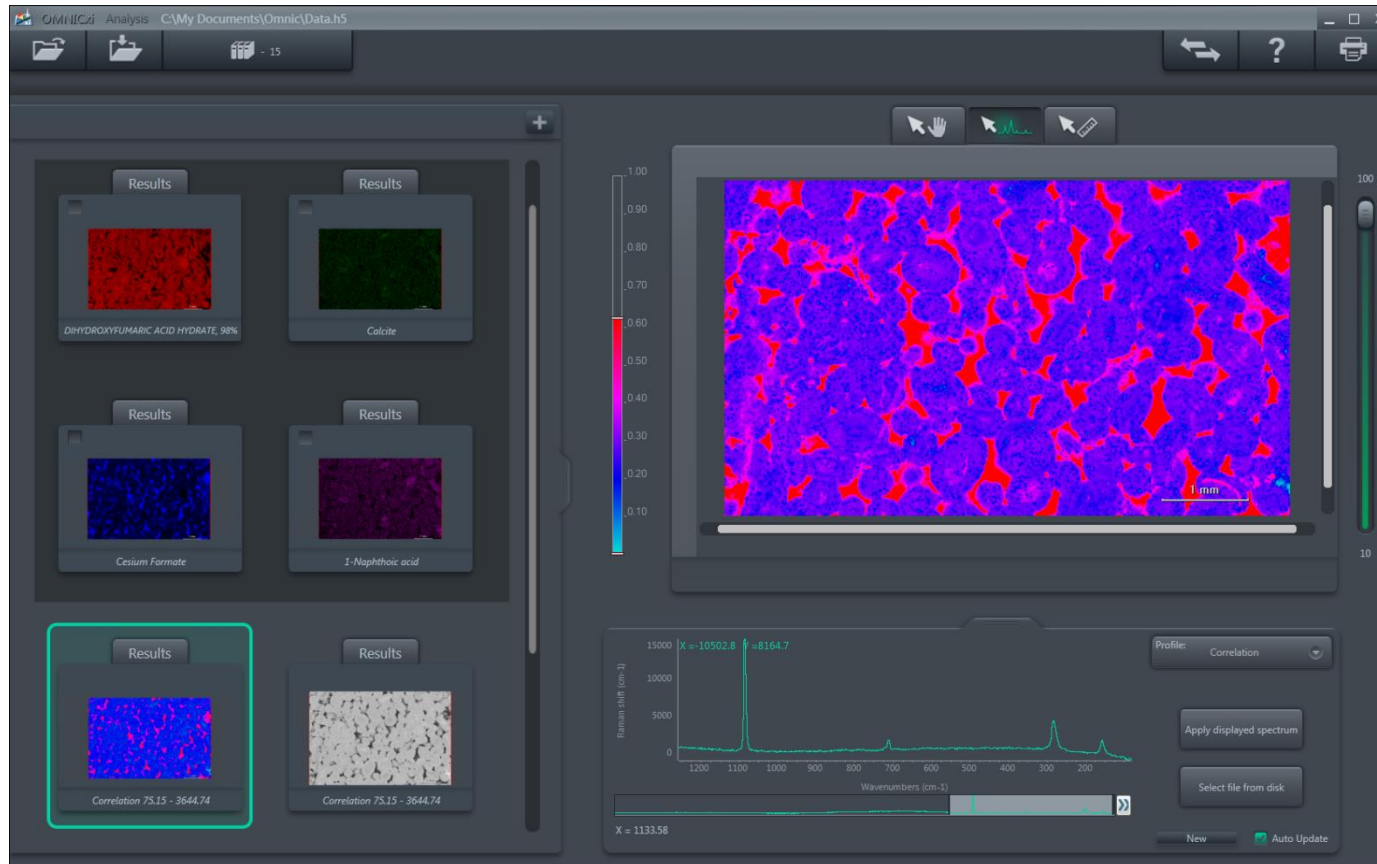


Sliders allow change of parameters on the fly to give immediate feedback

Simple, clean design is easy to navigate and visually striking

Image Centric Software: OMNICxi for Raman Imaging

Analysis window focuses on display of chemical image data

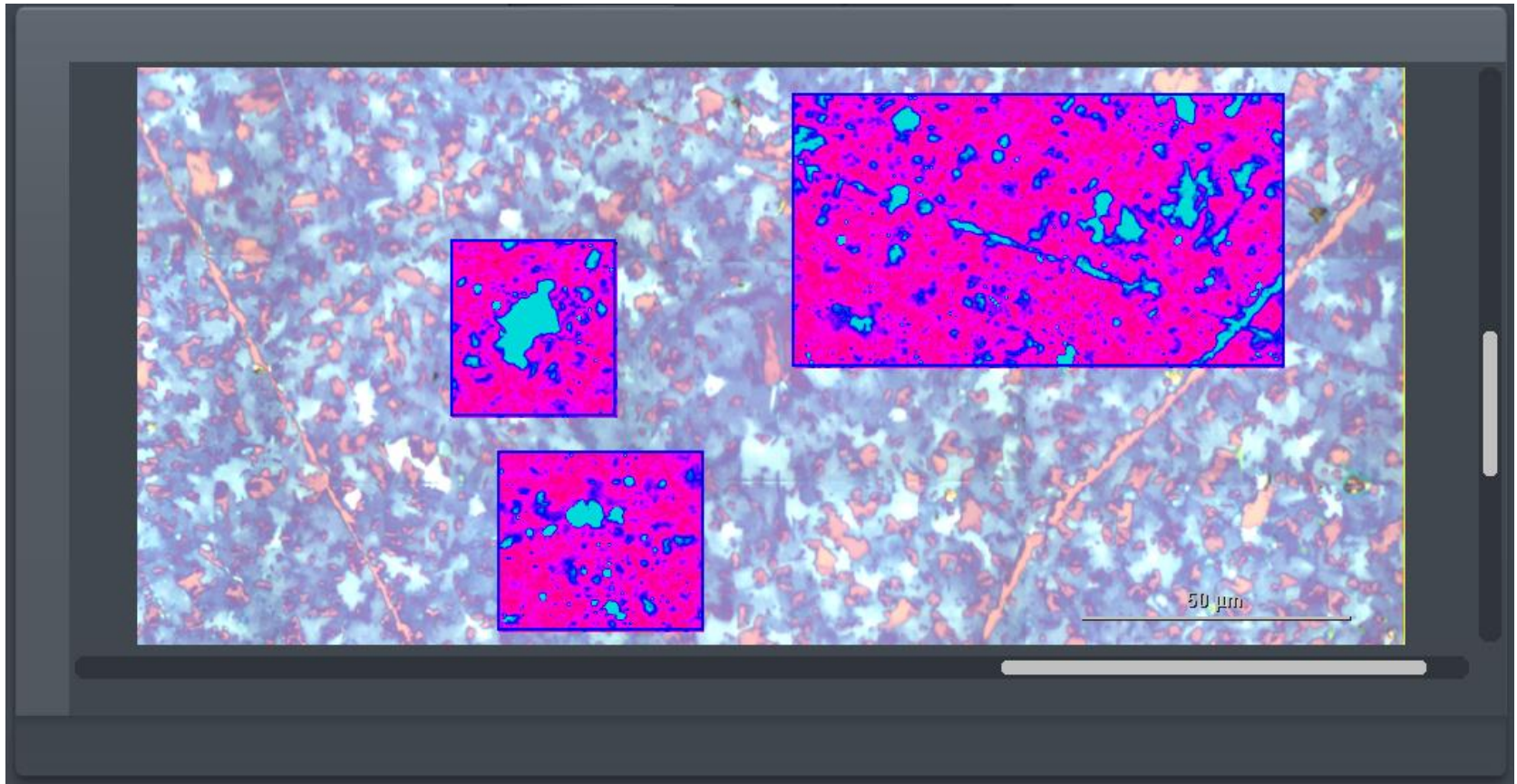


Profile thumbnails allow previous analysis to be applied in an instant

Spectra, MCR, and library search results displayed in familiar stacked format

Not Just Faster, Smarter: Multiple Collection Regions

- Why image an entire sample when several independent regions are really of interest?

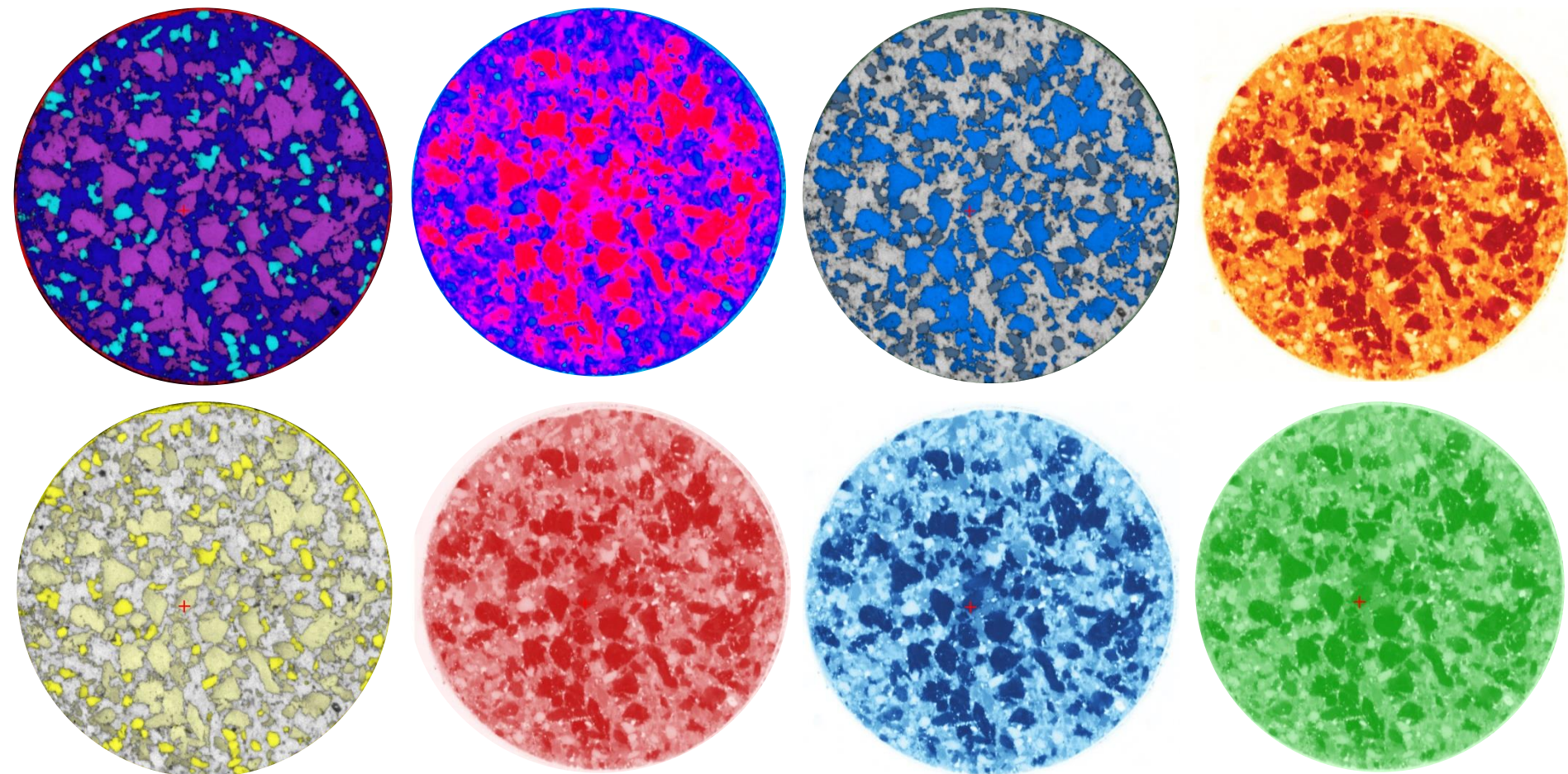


Cover your sample more efficiently to focus on what really matters

Producing Publication Quality Images: Colormaps

- User selectable color schemes enhance visualization of data

5 mm



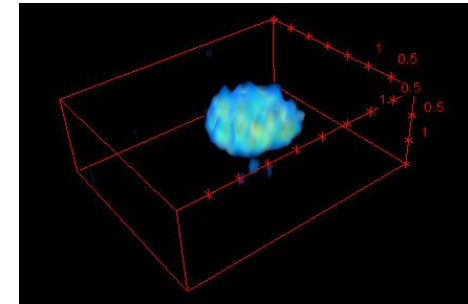
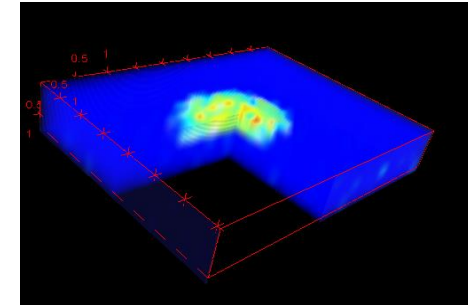
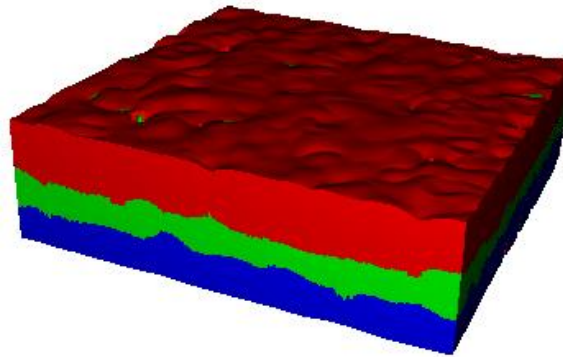
- Pharmaceutical tablet, 156,000 spectra with single scan collected in 8 min

Layer-by-layer Analysis for 3D Confocal Imaging

ID	Z Position	Width μm	Height μm
3	100	100	100
12	100.2	100	100
13	100.4	100	100
14	100.6	100	100
15	100.8	100	100
16	101	100	100
17	101.2	100	100
18	101.4	100	100
19	101.6	100	100
20	101.8	100	100

+ - Load regions Save regions Duplicate

Polymer multilayer with 5 μm spacing between imaging planes



Polystyrene bead on surface: full surface and 3/4 cutaway view

	# Duplicates	Offset μm
X		
Y		
Z	10	0.2

Duplicate Cancel

- Region queue also allows confocal imaging at different depths
- Provides same 3D data collection schemes as the competition!
- Also allows loading/saving list of regions
- Data can be easily exported to 3rd party packages

DXR Family Interchangeable and Upgradeable Components

- All DXR laser, filters, gratings, and microscopy accessories (objectives, sample holders, etc.) are compatible with the DXRxi
- Maximize value with shared components



Adaptability to any application, configurable by any user

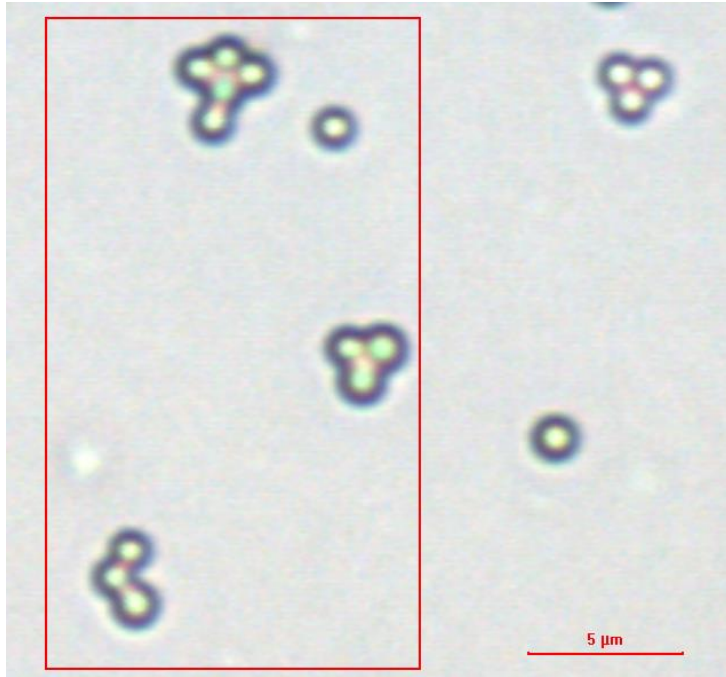
- Pre-aligned and lock-in-place components use automatic recognition and stored alignment, allowing any user to reconfigure an instrument in seconds
- Data standardization between excitation laser wavelengths
- Lasers and other components can be interchanged and shared with every instrument in the DXR Raman family





DXRxi Raman Imaging Microscope Key Applications

High Res Discrimination between similar 1 μm particles

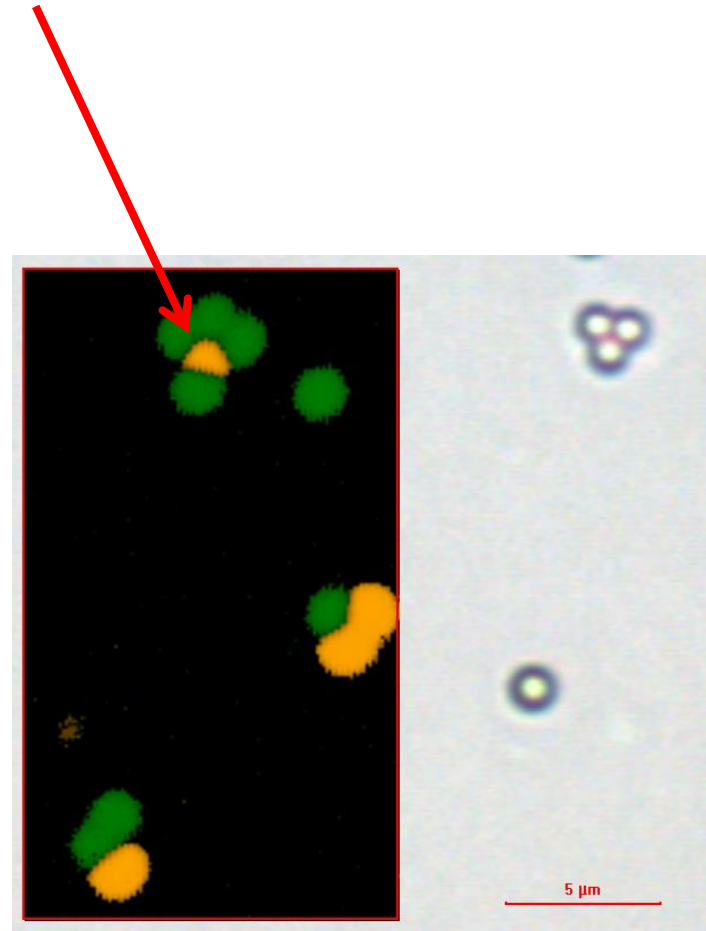


532 nm laser, 6.0 mW, 100X objective

25000 spectra, 0.1 μm pixel size

Acquisition parameters: 100 Hz (10 ms/spectrum),
20 scans

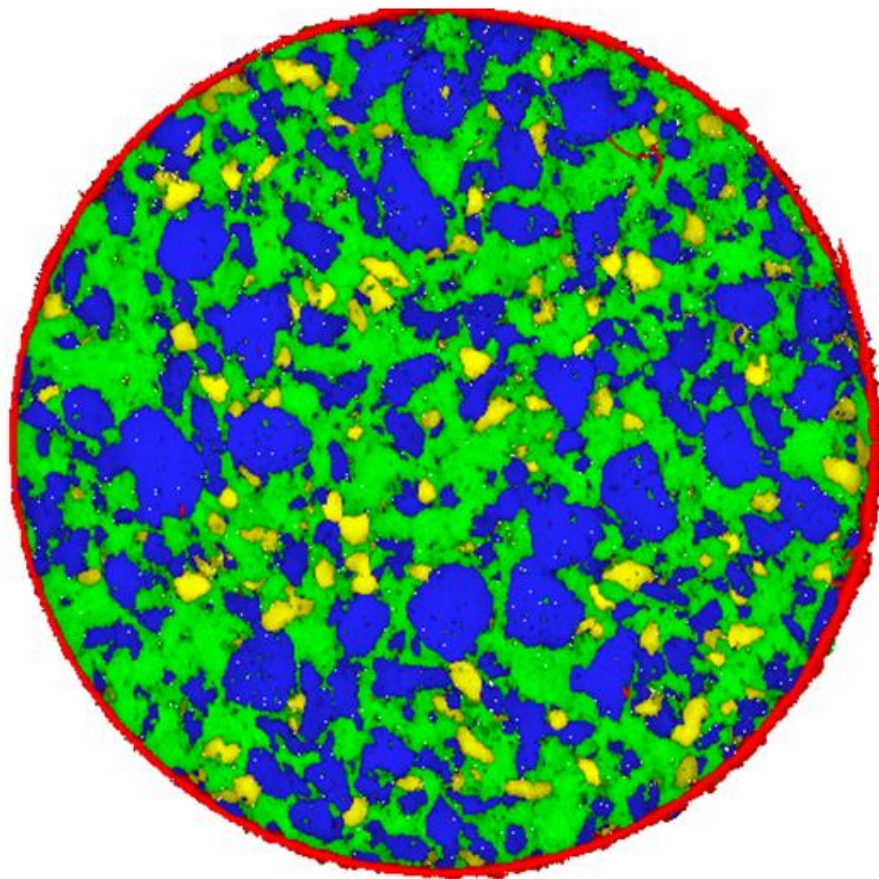
1.3 hr collect time



 Polystyrene  Polymethyl methacrylate

Surface Analysis of an Entire Headache Tablet

MCR Analysis



Determine:

- Size of each domain
- Distribution of domains
- Overall composition of tablet

11 x 11 mm surface area
532 nm laser, 10X objective

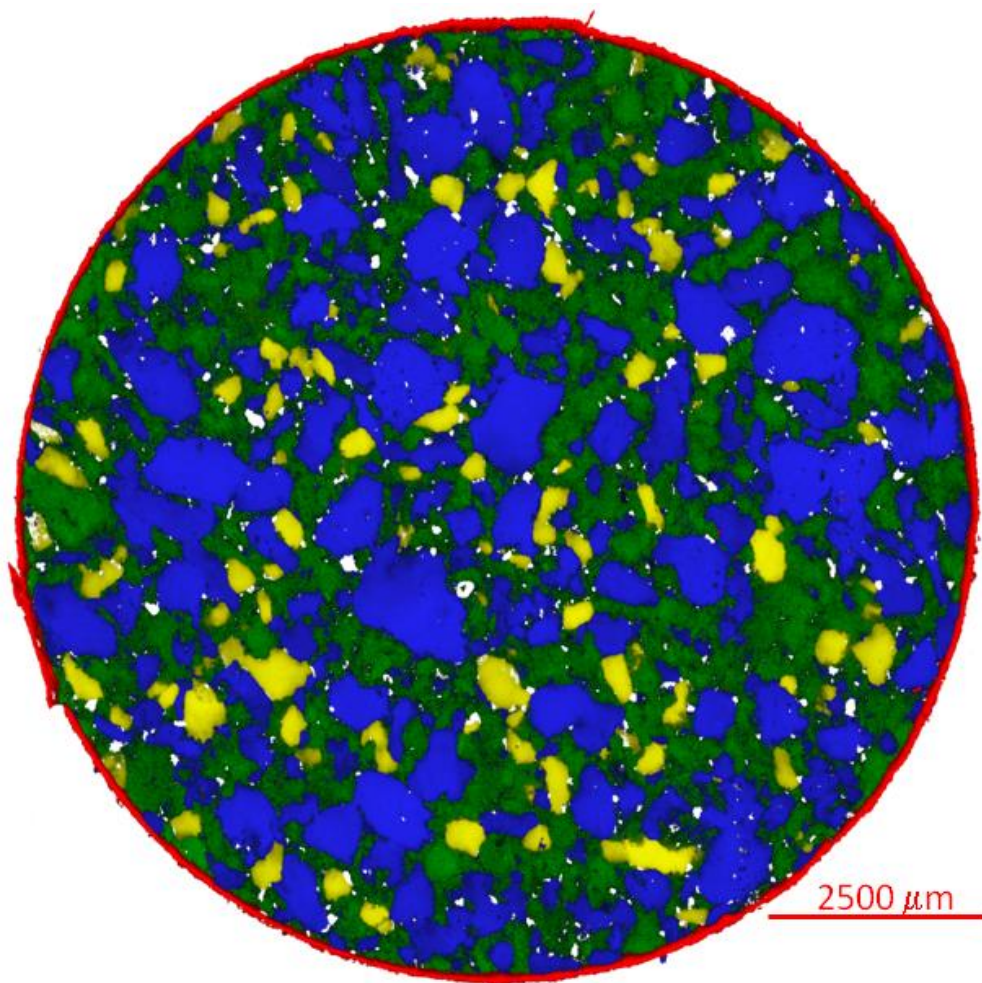
226,000 spectra, 25 μm pixel size

Acquisition parameters: 550 Hz (1.8
ms/spectrum)

8 minute collect time!!

■ Aspirin ■ Acetaminophen ■ Caffeine ■ Titanium Dioxide

Analysis of Pharmaceuticals



11 x 11 mm surface area
532nm laser

5.4 million spectra!!!

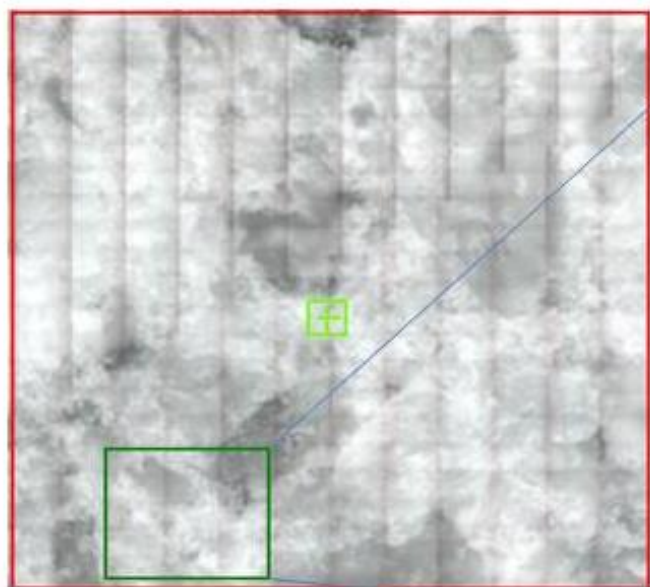
0.5 μm pixel size
Acquisition parameters: 550 Hz
(1.8 ms/spectrum)

~3 hour collect time!!

Component	Calculated % (Surface Area)	Reported %
Aspirin	38.6	37
Acetaminophen	35.4	37
Caffeine	7.7	9.6

■ Aspirin ■ Acetaminophen ■ Caffeine ■ Titanium Dioxide

High Resolution MCR Analysis of Pharmaceuticals

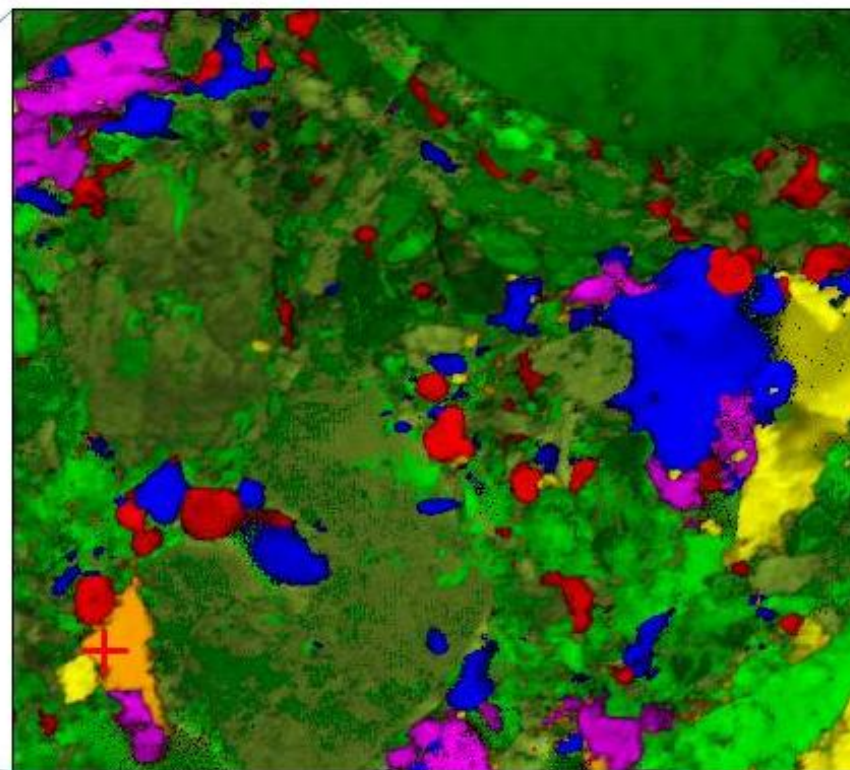


500 μm

225 x 250 μm surface area
532nm laser, 100X objective

229,000 spectra, 0.5 μm pixel size
Acquisition parameters: 100 Hz (10
ms/spectrum)

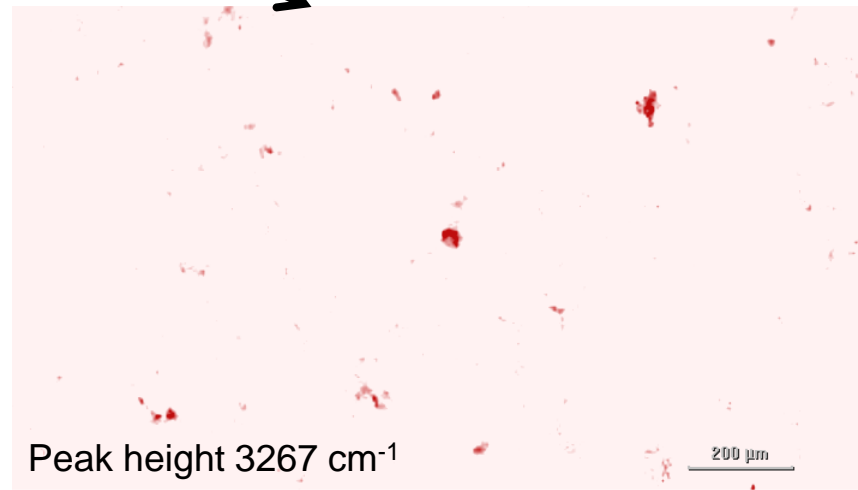
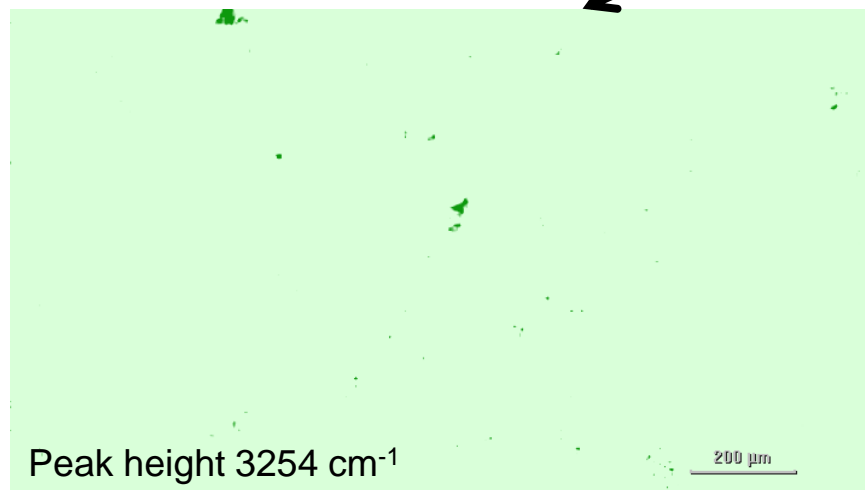
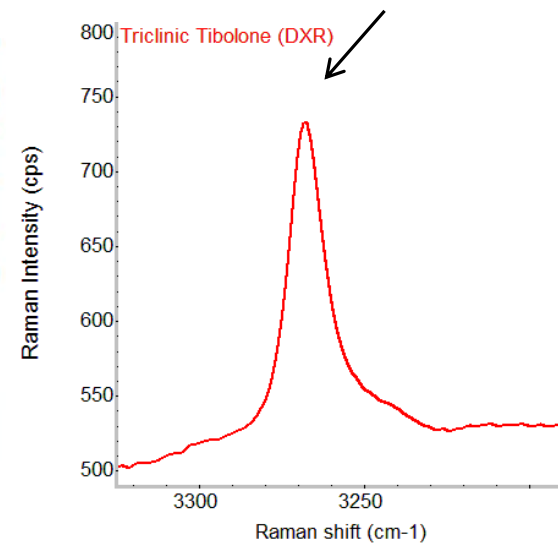
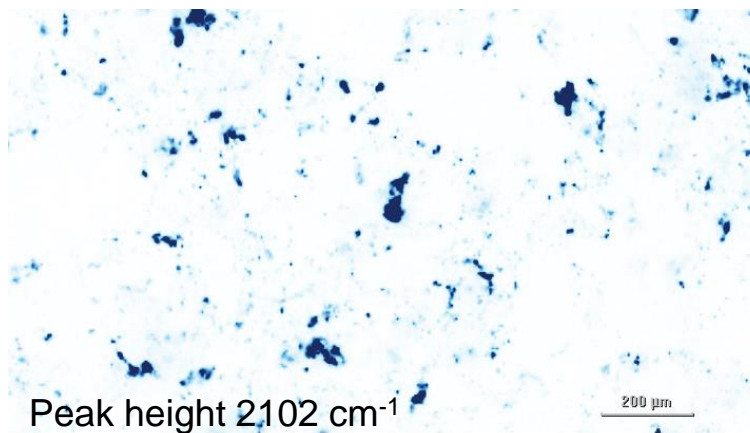
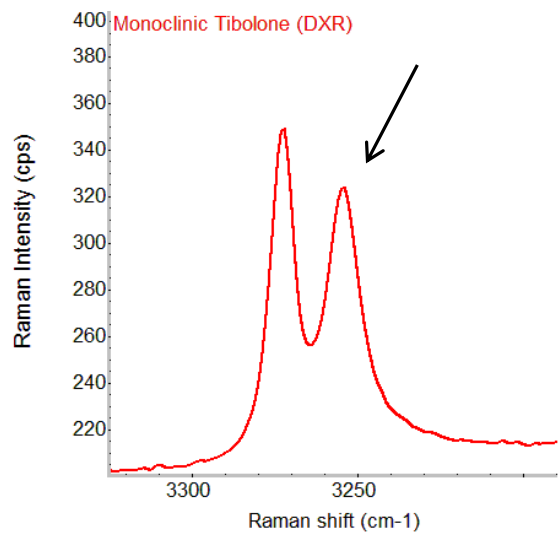
3 hour collect time!!



100 μm

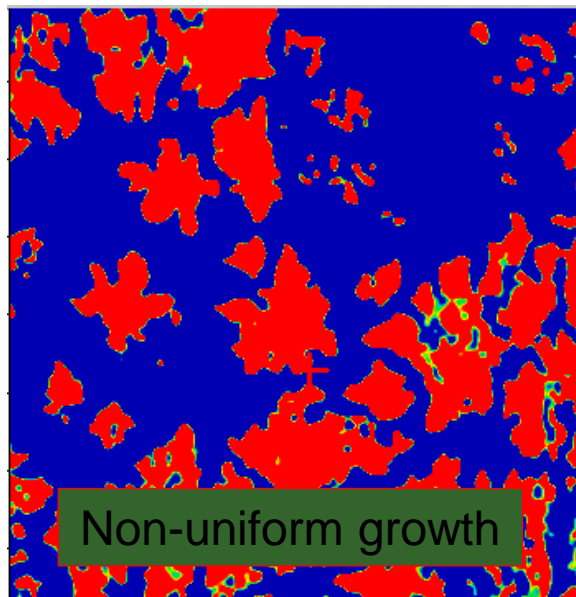
■ Aspirin ■ Acetaminophen ■ Caffeine ■ Starch
■ Microcrystalline Cellulose ■ Sodium Lauryl Sulfate

Polymorph distribution of Tibolone



Analysis of Graphene, 532nm laser

Ratio of the 2D to G band of graphene:



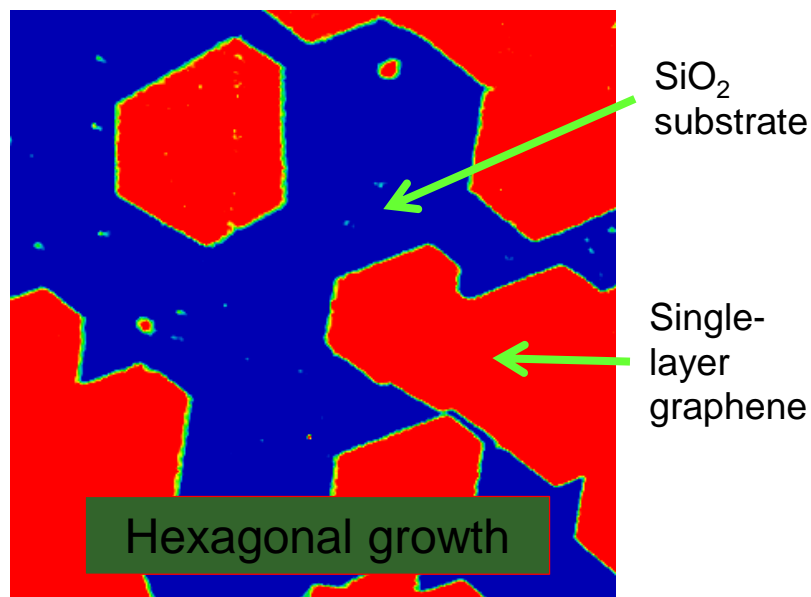
50 x 50 μm surface area

10,000 spectra!!!

Acquisition parameters: 100 Hz (10 ms/spectrum)

~16.7 minute collect time!!

MCR of graphene:



175 x 175 μm surface area

122,000 spectra!!!

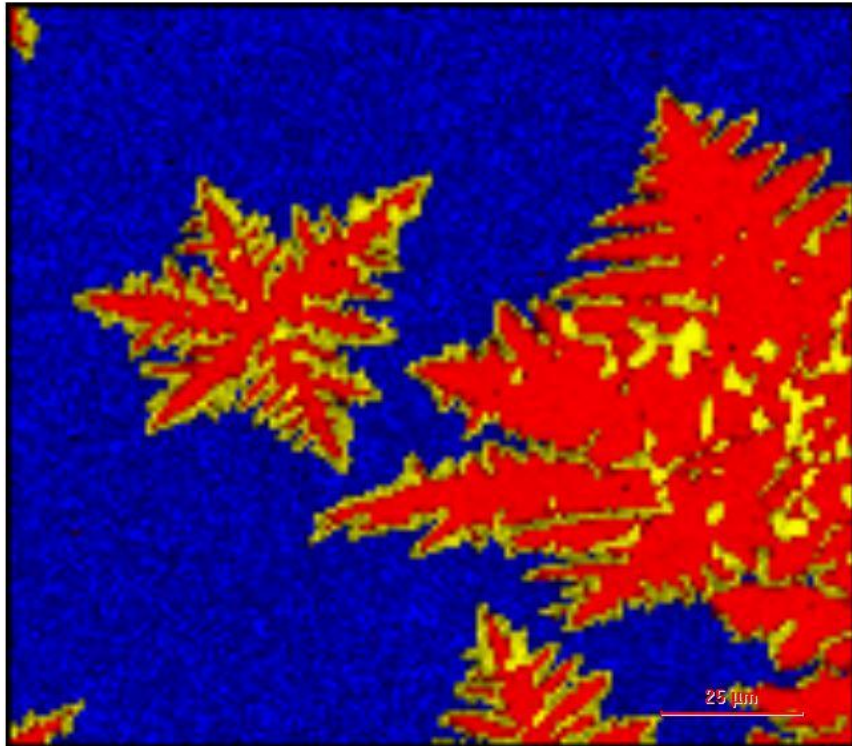
0.5 μm pixel size

Acquisition parameters: 100 Hz, 10 scans

~3.4 hour collect time!!

*Note: This graphene was initially grown on copper and then transferred to a silica substrate because the copper is a significant source of interference

Analysis of Graphene on a Copper Substrate



Graphene grown on copper and analyzed **on the copper** with the 455nm laser

$$I_{scatter} \propto \frac{1}{\lambda_{ex}^4}$$

455nm laser

150 x 150 μm surface area

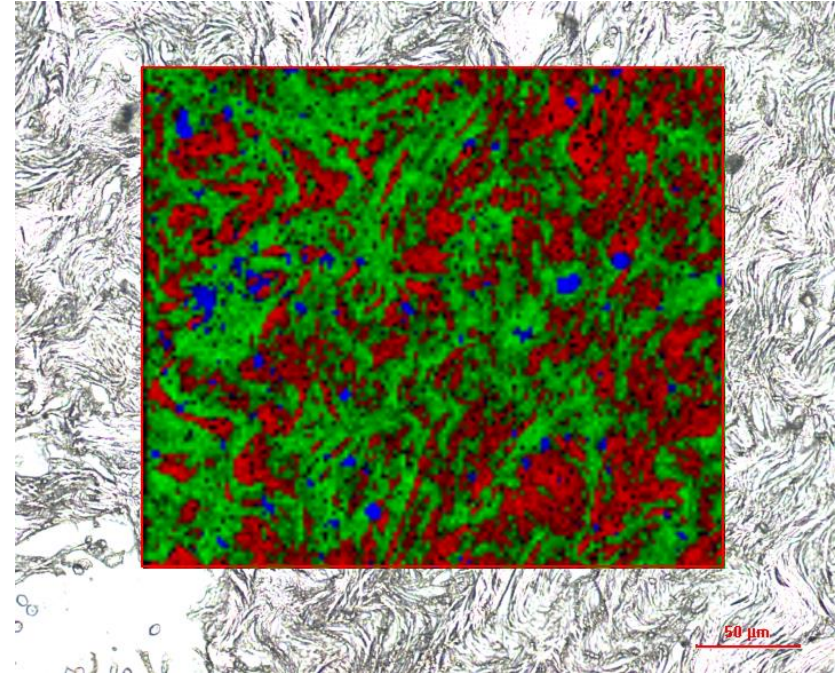
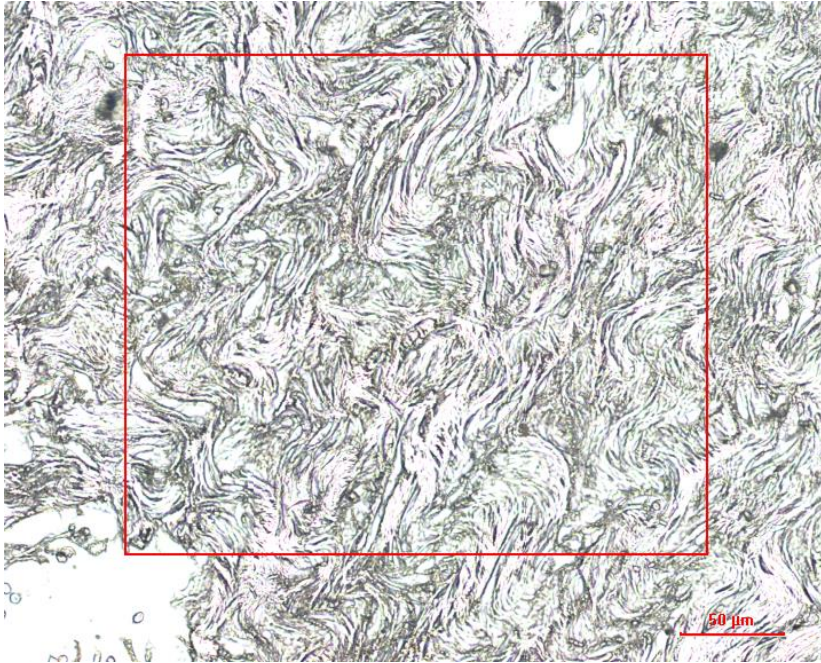
90,000 spectra!!!

2.0 μm pixel size

Acquisition parameters: 100 Hz (10 ms/spectrum),
4 scans

■ Copper Substrate ■ Oxidized Copper ■ Single-layer graphene

Analysis of Normal Breast Tissue



532 nm laser, 5.4 mW, 50X objective
17,000 spectra

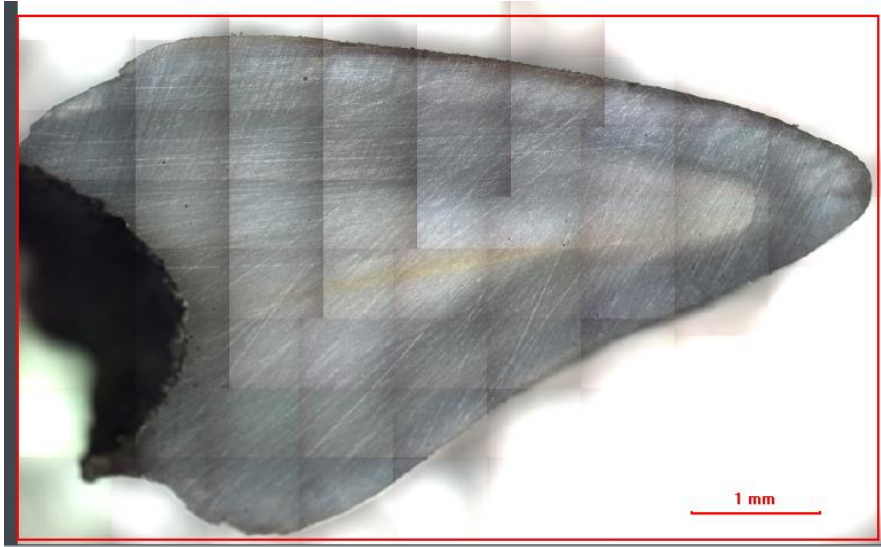
Acquisition parameters: 40 Hz (25 ms/spectrum),
100 scans, 2.0 μm pixel size

■ Cell Nuclei ■ Collagen ■ Glass Slide

~13 hour collect time!!

Sample provided by Ihtesham ur Rehman, University of Sheffield

Analysis of Human Teeth



780nm laser, 5.9 mW, 10X objective

29,000 spectra!!!

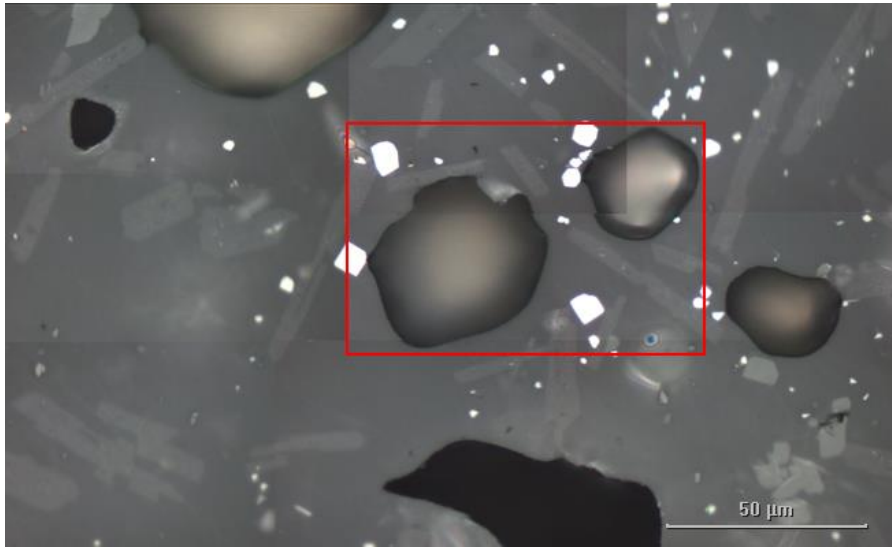
Acquisition parameters 40 Hz (25 ms/spectrum),
100 scans, 30 μ m pixel size

~22 hour collect time
Impossible on a traditional
mapping instrument!



■ Pulp ■ Circumpulpal Dentin ■ Dentin ■ Enamel

MCR Analysis of Synthetic Volcanic Rock-Volatile Analysis



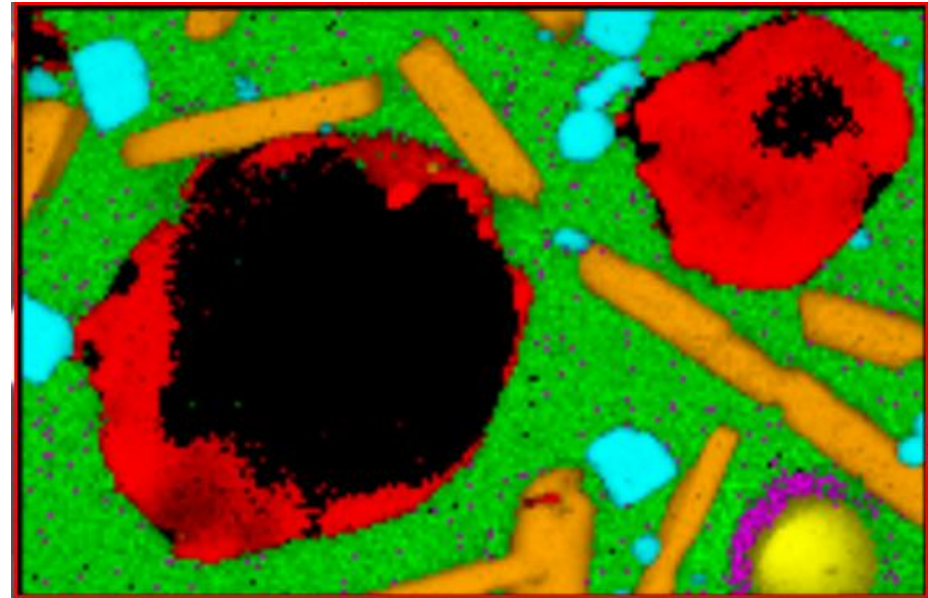
455 nm laser, 5.9 mW, 100X objective

21,000 spectra

Acquisition parameters: 40 Hz (25 ms/spectrum),
100 scans, 0.5 μm pixel size

The DXRxi maintains the same confocal capability as the DXR

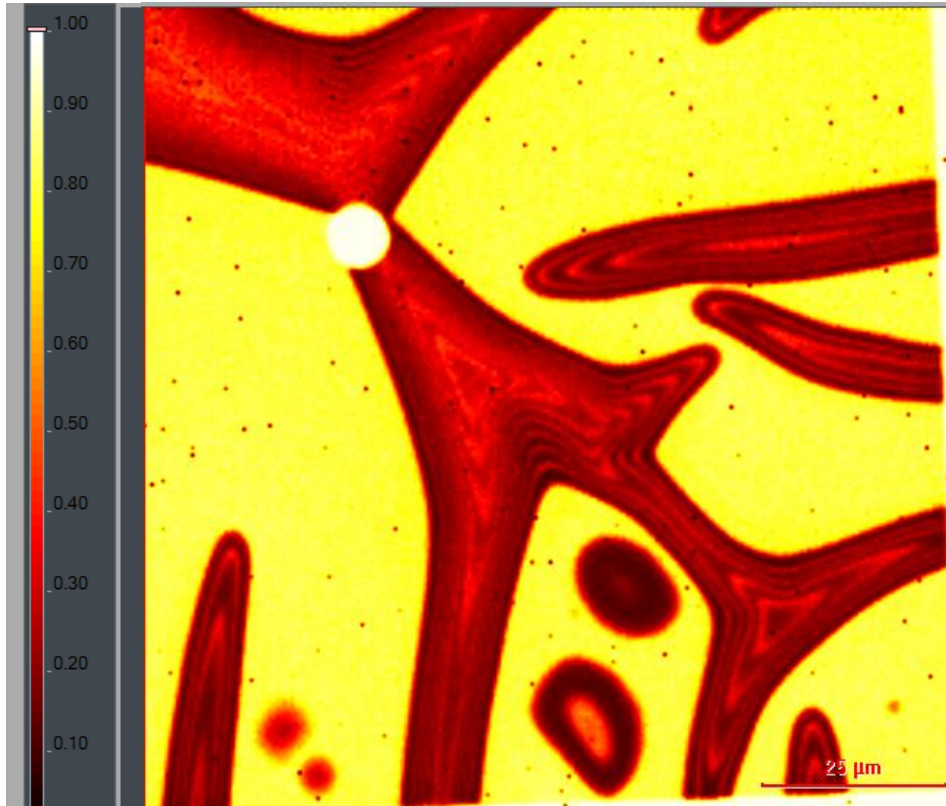
Quantifying the volatiles in the sample will provide clues about the nature of volcanoes.



■ Glass ■ CO₂ ■ Carbon ■ OH
■ Chalcocite? ■ Labradorite?

Sample provided by Jenny Riker, University of Bristol

Analysis of Stress in Silicon—Correlation Image



455 nm laser, 1.0 mW, 100X objective

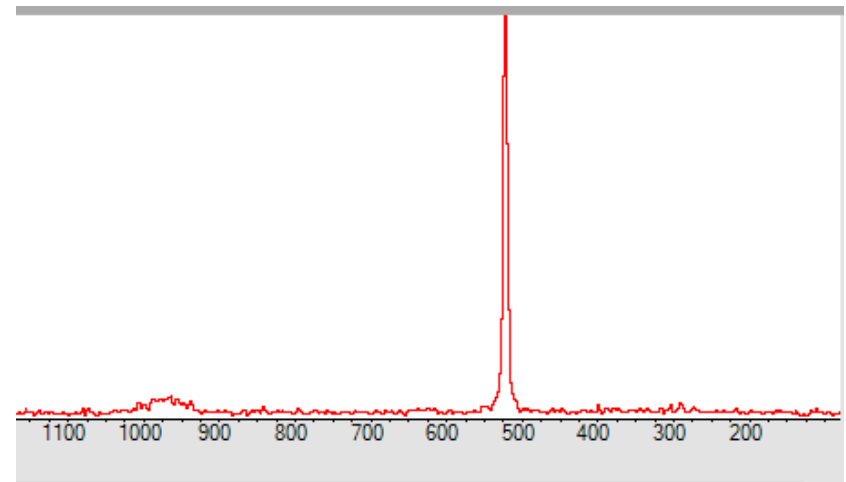
50,000 spectra

Acquisition parameters: 100 Hz (10 ms/spectrum),
25 scans, 0.5 μm pixel size

~4 hour collect time!!

Sample is a Si substrate with a layer of Si/Ge deposited followed by an additional layer of Si

The presence of the Ge causes stress in the second layer of Si, which is imaged





ThermoFisher
S C I E N T I F I C

DXRxi Raman Imaging Microscope Who needs one?

- Strong organizational value for **academic** and **industrial** users



Interdisciplinary Academic Research Laboratories

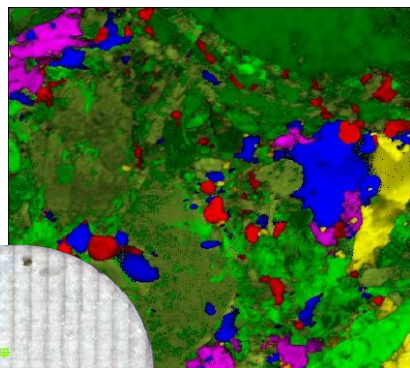
- Allows multiple users to focus on their research, not the technique
- Simple operation accommodates users of all skill levels
- Enables rapid progress in the new research directions you want to take



Industrial Research and Product Development

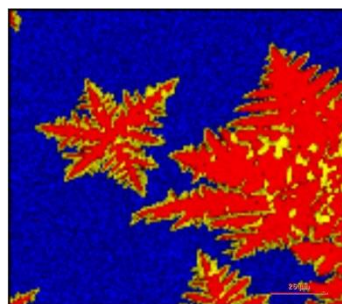
- Designed from the ground up to ensure stable results and confidence in your data
- Intuitive workflow maximizes throughput for the most demanding applications
- World-class service and support keeps you running around the clock

- Key application areas for leveraging performance and ease of use:

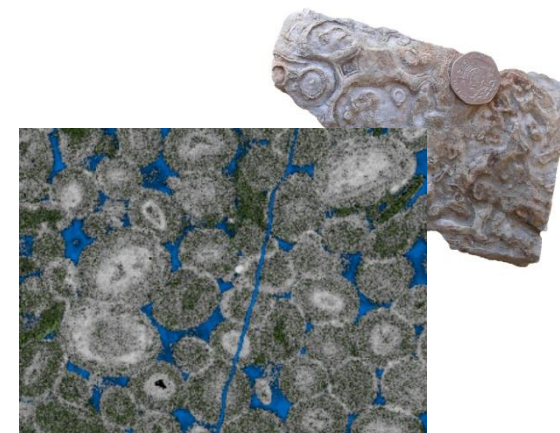
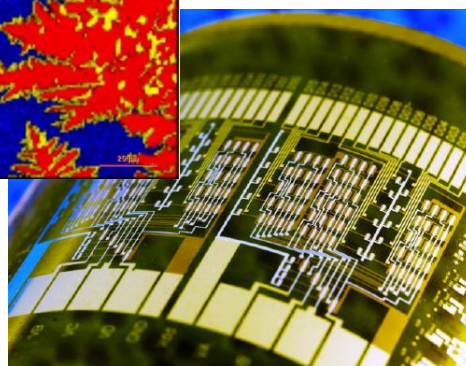


100 μm

PHARMA



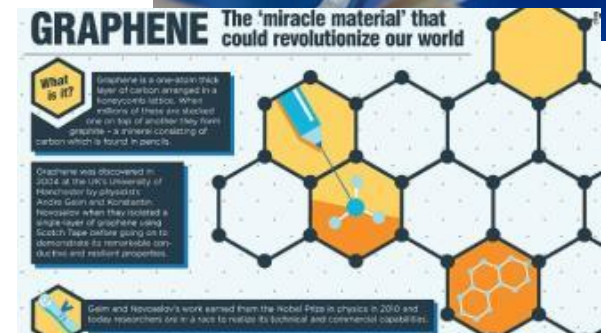
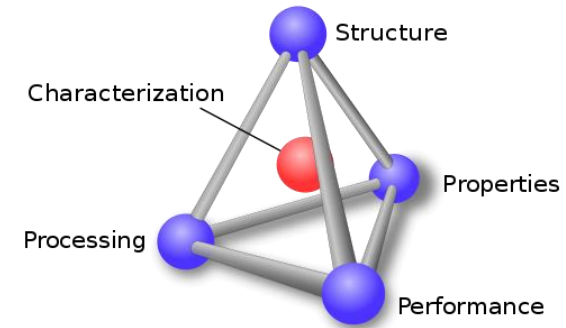
ADVANCED MATERIALS



GEOLOGY / MINERALOGY

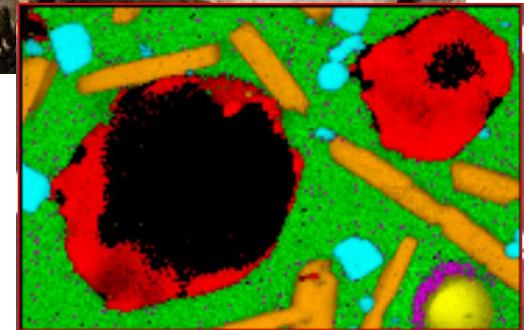
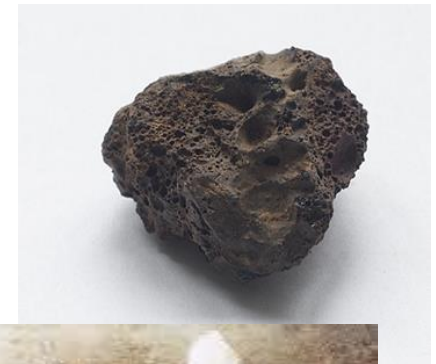
Example User #1: Materials Science Researcher

- Market: Academia and Industry
- Example User: Materials science researcher
- Example Field of Study: Growth processes, functionalization, and applied uses of graphene and other nanomaterials; moving from characterization to real-world applications
- Key needs/points: Need broad understanding of structure-property relationships. Many tools used in complementary fashion, offered shared among groups/departments. Main expertise is at domain level – not in Raman.
- What the DXRxi provides:
 - A microscopy-first approach to Raman imaging, that quickly rasters across a sample like an AFM/SEM
 - Profiling tools show differences and allow image refinement to features and components of interest without having to know or understand Raman
 - High sensitivity to graphene and other advanced materials
 - High fidelity between optical and chemical image from data triggering technology
 - High approachability without specific Raman expertise



Example User #2: Earth Science Research Group

- Market: Academic Research Group (1-2 Principal Investigators)
- User: graduate student, postdoctoral researcher, or scientist
- Application(s): mineral identification, study of inclusions, characterization of physical properties (pressure, phase/morphology)
- Key needs/points: Used for a diverse range of projects by users who are experts in their own research/sub-field. Sample dimensions and features vary widely, from large areas to micron-scale inclusions. Identification of unknowns is key. Experiments may be extremely simple (“what is it”) to very complex (“how did it evolve over time”).
- What the DXRxi provides:
 - Walk-up ease of use to reduce training requirements
 - Broad range of sampling stage options for many different sample types
 - Rapid identification with integrated library searching
 - Exceptional optical targeting and competitive spatial resolution to isolate small defects/inclusions



Example User #3: Multi-User Labs in Academia

- Market: Interdisciplinary academic labs
- User: graduate student, postdoctoral researcher, or scientist
- Application: Broad range of problems coming from many different departments/disciplines
- Key needs/points: Research applies Raman as a tool – doesn't focus on developing the technique. Labs accessed by hundreds of different users, each with a unique set of research goals
- What the DXRxi provides:
 - Stable and reliable operation to ensure confidence in the data and unambiguous results
 - Consistent user experience: easy to configure, easy to maintain
 - Flexible software workflow allow experiments to be conducted in many different ways
 - Expertise built-in to minimize time spent in data interpretation

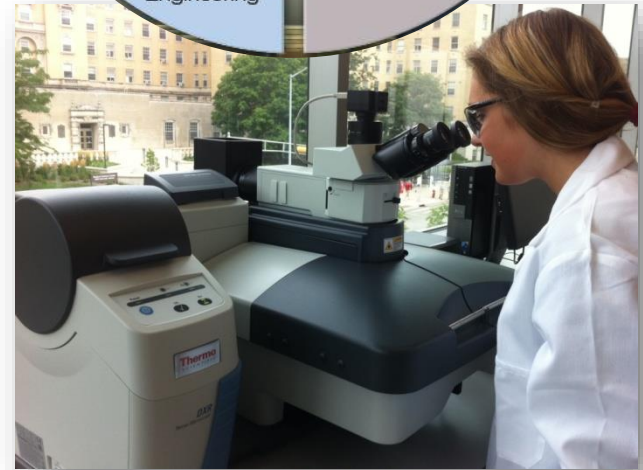
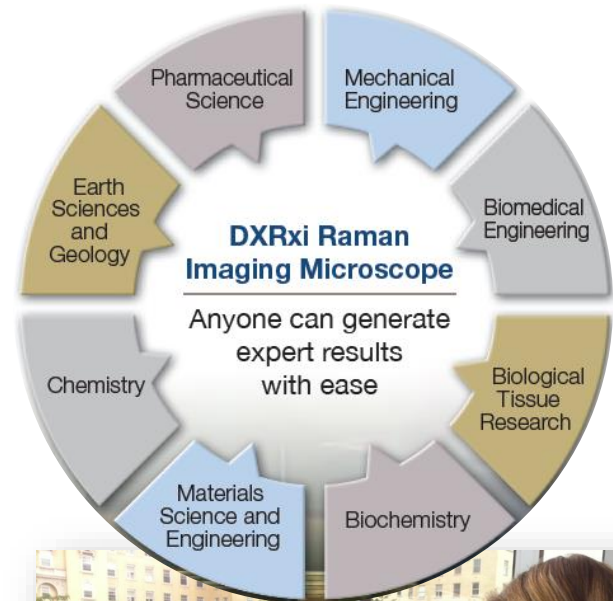
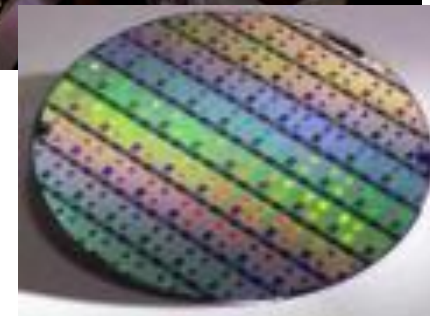
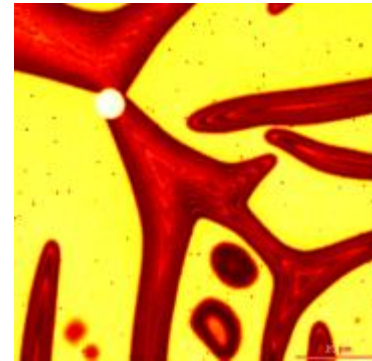


Photo courtesy of University of Wisconsin-Madison

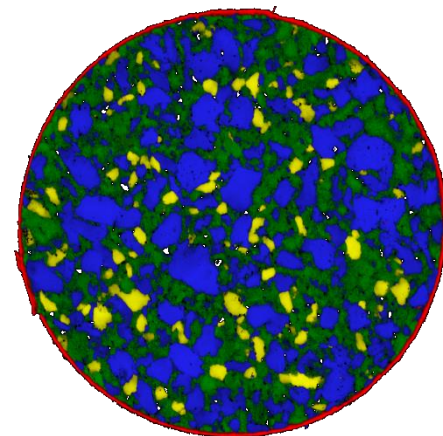
Example User #4: R&D/ Analytical Support

- Market: Semiconductor/Electronics
- User: Process and product support scientist
- Application: Hard disk coating inspection and defect/contaminant analysis
- Key needs/points: Competitive industry and need to solve problems quickly with very high precision. Need to look at both chemical and physical information such as crystallinity, coating thickness, and uniformity. Submicron defects and contaminants are essential to find and identify.
- What the DXRxi provides:
 - Very fast rastering and real-time statistical processing to locate the invisible “needle in a haystack”
 - Large area scanning or multiple region collection with ability to save and load standard set of parameters
 - Fast reliable image preview and real-time correlation analysis rather than waiting for measurements to finish
 - Strong global support team and reliable design



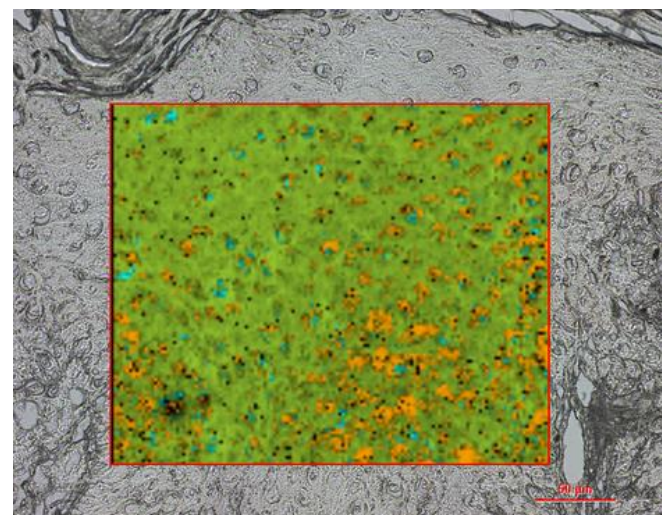
Example User #5: Pharmaceutical Scientist

- Market: Pharmaceuticals
- User: Scientist in formulation development
- Application: Solid dosage form product and process development including new hot melt extrusion processes
- Key needs/points: Understand entire dosage form, including distribution of components and relative concentrations. Spot unexpected components/contaminants without knowing they are there, identify them with confidence. May need to see subtle polymorphism effects. Tablets can have hundreds of times the area of the field of view. Users may be spectroscopists but must be efficient to support product development and are interested in the big picture of a batch of tablets quickly.
- What the DXRxi provides:
 - Rapid chemical imaging of entire tablets and other solid dosage forms
 - Real-time identification of chemical components, approximate concentrations, and visual confirmation of distribution and uniformity
 - Strong pharmaceutical libraries and real-time identification for targeting of sample areas
 - Auto alignment and simple controls that facilitate repeatable results
 - Whole table imaging with single stage, single mode collection and continuous chemical imagery

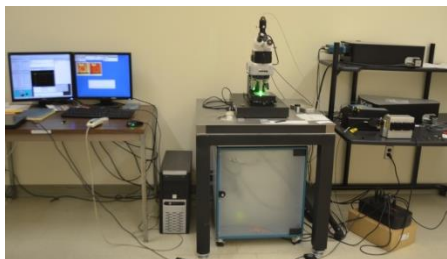


Example User #6: Biological/Life Science

- Market: Academia
- User: Biological/Life Science researcher
- Field of Study: Disease processes, diagnostics
- Key needs/points: Strong users of light microscopy and good acceptance of FTIR imaging for research. Research growing from areas with spectroscopic expertise, but current mapping methods are extremely slow and resolution is limited. Samples are biological and sample preparation and manual staining are the normal process. Spectroscopic need is finding differences and isolating spectral signatures of disease.
- What the DXRxi provides:
 - Visual approach similar to light microscopy
 - Automatic recognition of visual features to target analysis
 - Spectral tools to refine image rapidly to pull out details of interest, and spectroscopic “staining” to replace or complement tedious manual diagnostics
 - Better discrimination than visible microscopy, less sample preparation and higher resolution than FTIR



Performance: Total Experiment Time



**Typical
“research
Raman”
instrument**

**DXRxi Raman
imaging
microscope**



Configure Instrument	0.5 - 2 DAYS	8 - 10 MINUTES
Align & Calibrate	1 - 4 HOURS	5 - 10 MINUTES
Mount & Target Sample	1 - 60 MINUTES	1 - 10 MINUTES
Optimize Parameters	5 - 20 MINUTES	1 - 2 MINUTES
Collect & Process Data	3 - 20 MINUTES	5 MINUTES - 2 HOURS performed in real-time – as little as a few minutes
Interpret Data	0.5 - 2 DAYS	1 - 2 MINUTES
Apply Results	5 - 20 MINUTES	



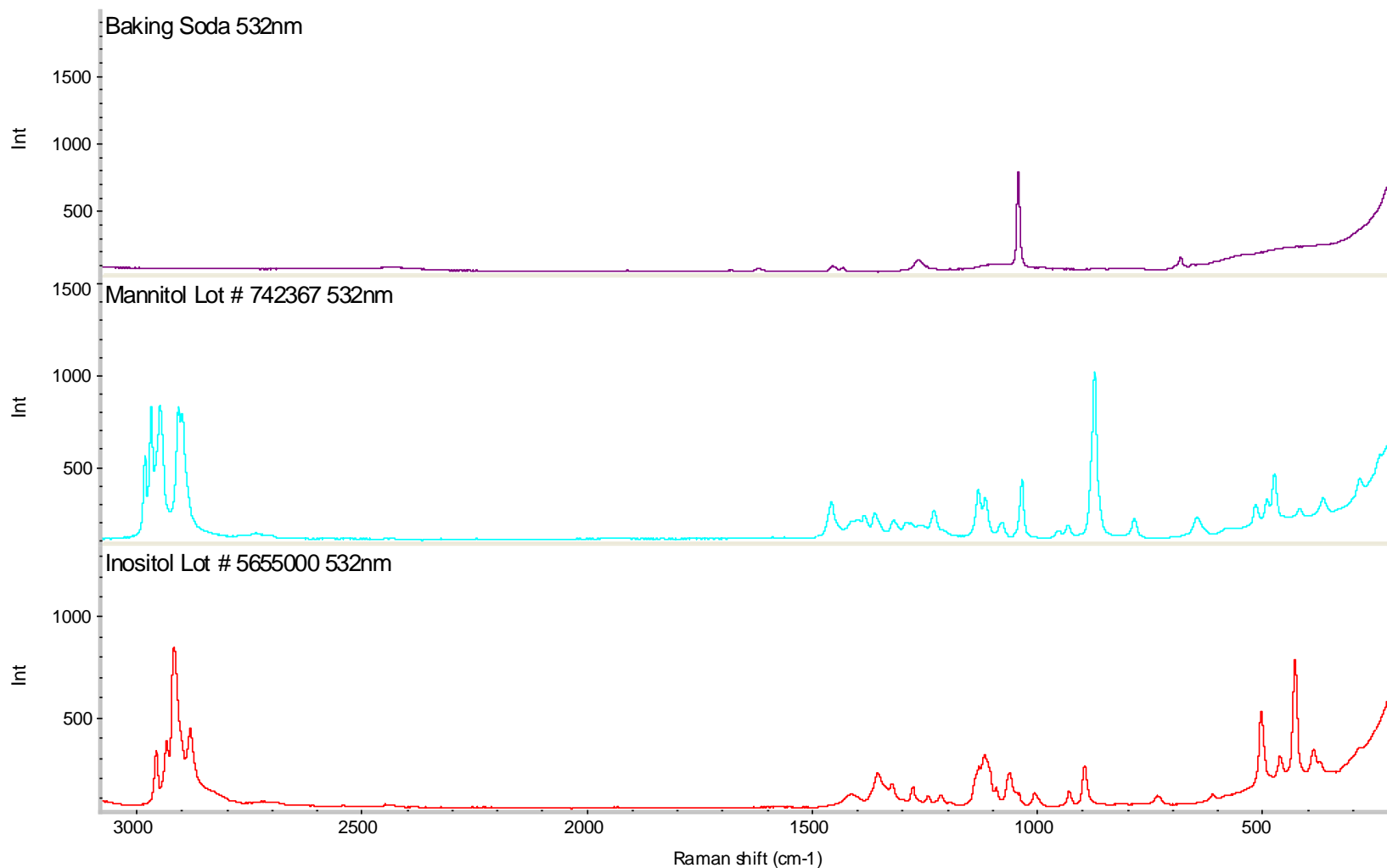
Ease of Use Has BIG Impact on Reducing Time to Answers

Why Raman Microscopy in Forensic Science

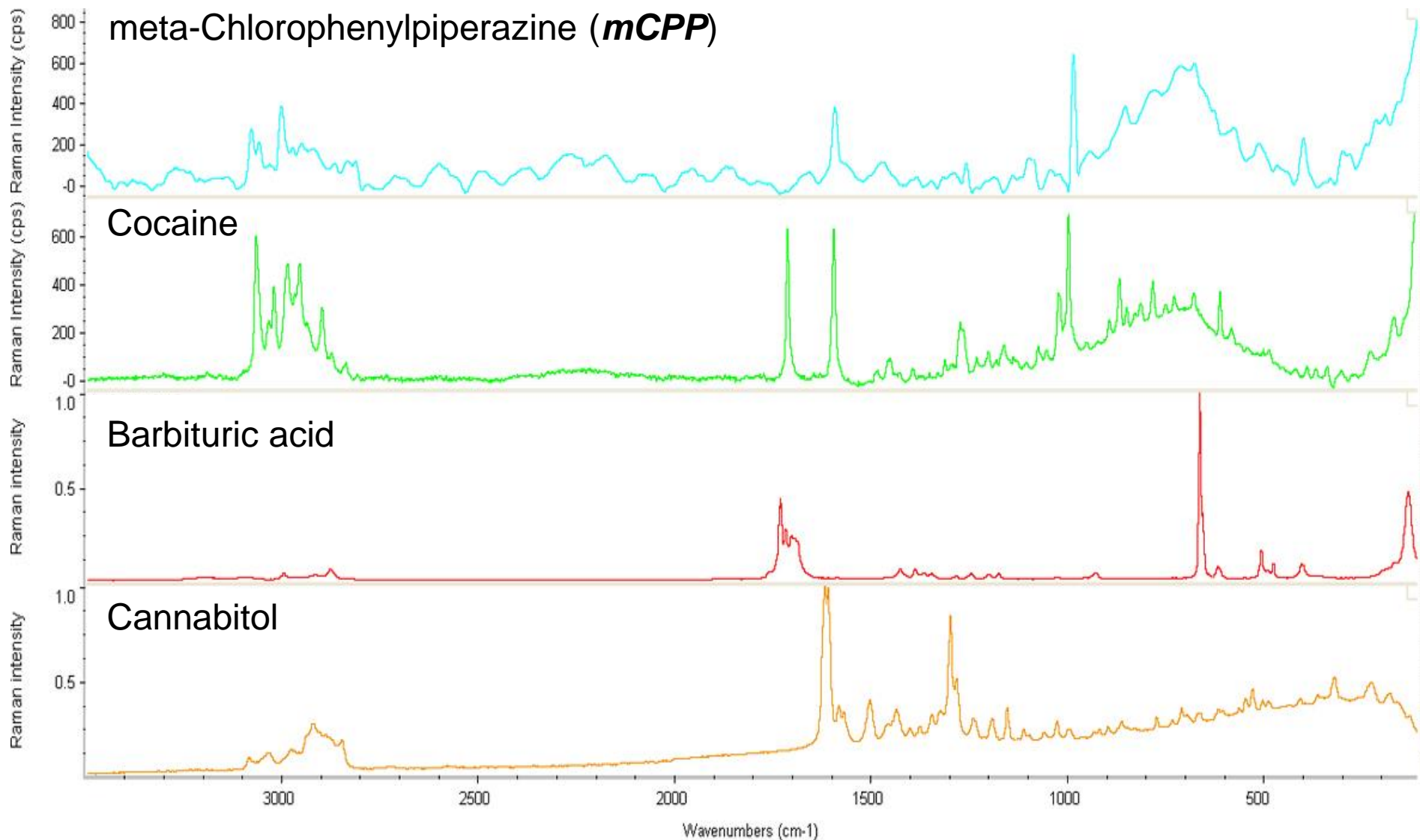
- Small particle size collection - down to 1 μ m
- Virtually no sample preparation – particle isolation only
- Non destructive
- Extended spectral range to 50 cm^{-1}
- Inorganic and organic identification
- Quick sample collection
- Complementary to FT-IR
- Very sharp spectral features
- Confocal Analysis → Sample through glass, plastic
- No Atmospheric Interference
- No water interference
- Small analytical volume ensures spectral purity

Substances Abuse Identification Cutting agent

- Cutting Agents



Substances Abuse Identification Illicit drugs



Substances Abuse Identification



DIFFERENT DRUG PARTICLES

A dashed orange line connects the central text box to the two images below.



**FINGERPRINT
LIFTING TAPE**



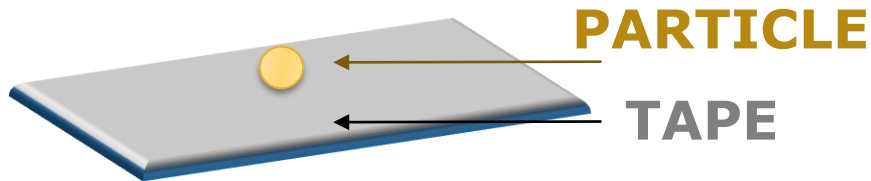
**WHITE AND GREEN
PACKAGING TAPE**

Substances Abuse Identification

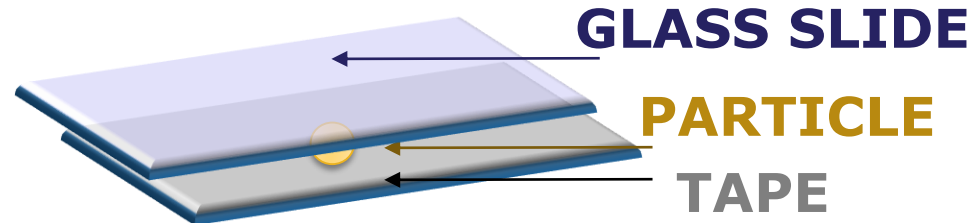
DIFFERENT DRUG PARTICLES



PARTICLES ON TOP OF THE TAPES



PARTICLES TRAPPED BETWEEN GLASS SLIDE AND TAPE



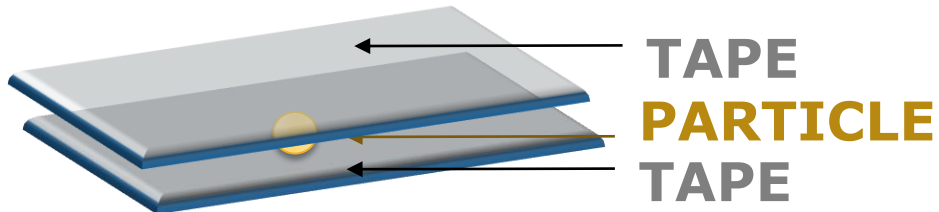
Substances Abuse Identification



DIFFERENT DRUG PARTICLES



**PARTICLES IN THE TAPE
FOLDED OVER ITSELF**



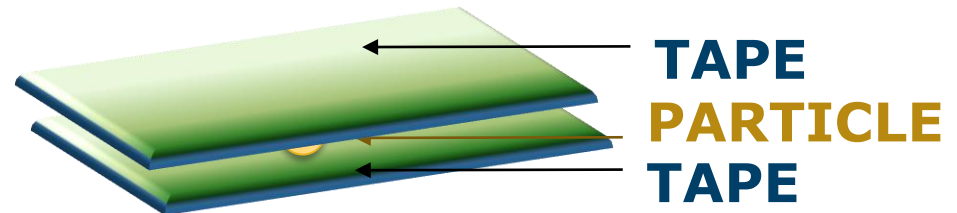
Substances Abuse Identification



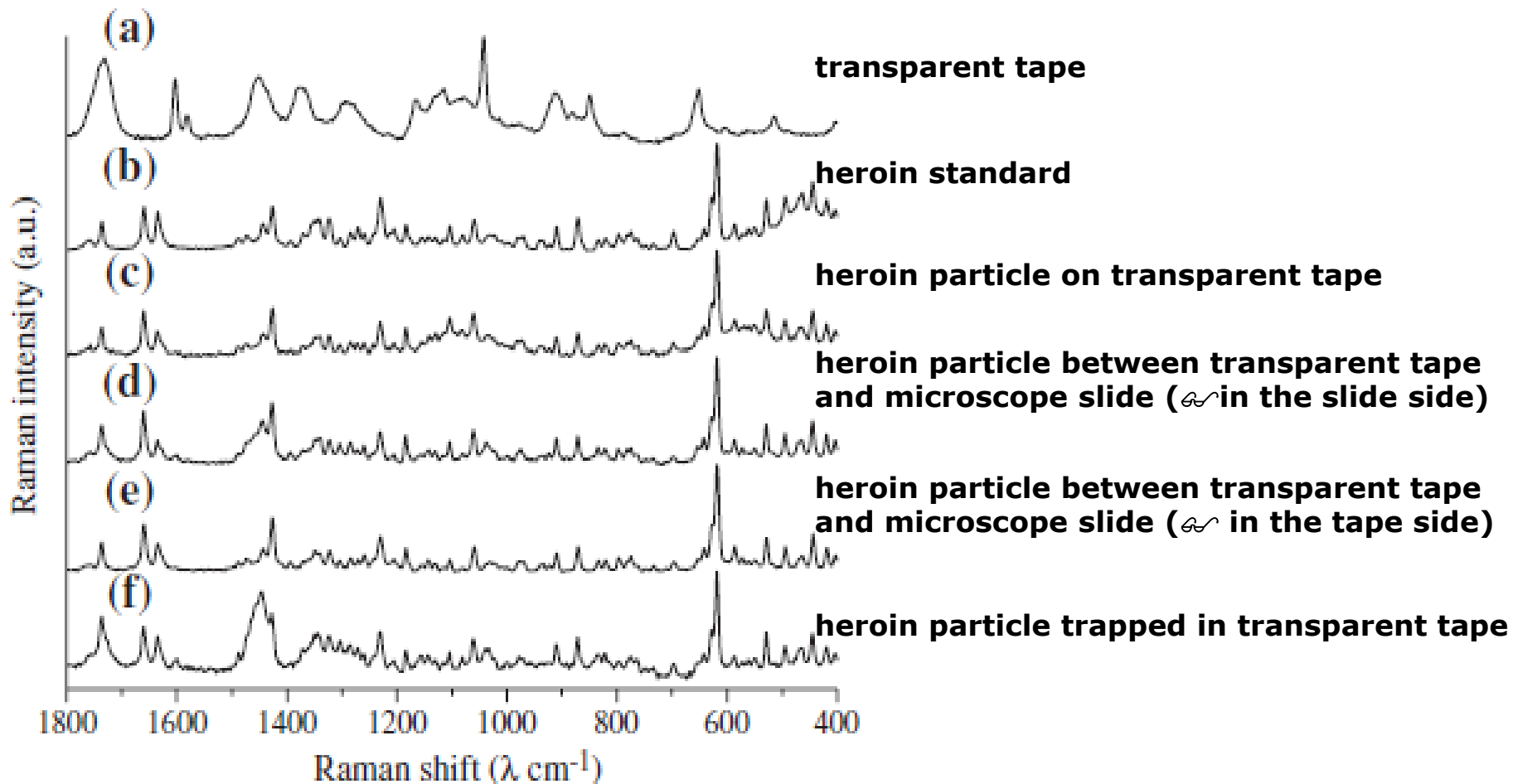
DIFFERENT DRUG PARTICLES



AFTER FOLDING AND UNFOLDING THE TAPE



Substances Abuse Identification



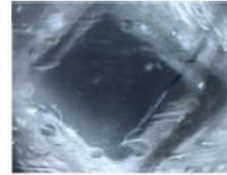
Magnification objective lens: 10 \times (a–b) and 20 \times (b–f). Spectral acquisition time: 1 s \times 50 acquisitions. Laser power: 10.0 mW.

Substances Abuse Identification

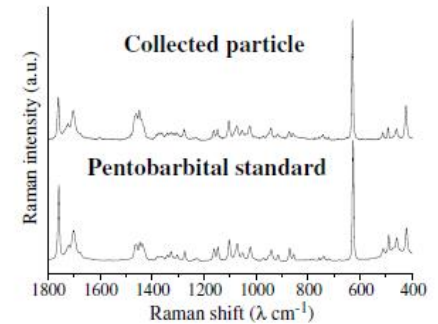
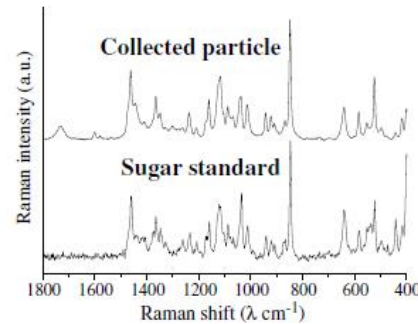
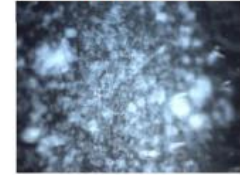
Illicit drugs on a clean table

Magnification objective lens: 10× for standards and 20× for particles.
Spectral acquisition times: 1 s × 50 acquisitions (particles 1–4 and drug standards) and 1 s × 10 acquisitions (sugar standard). Laser power: 10.0 mW.

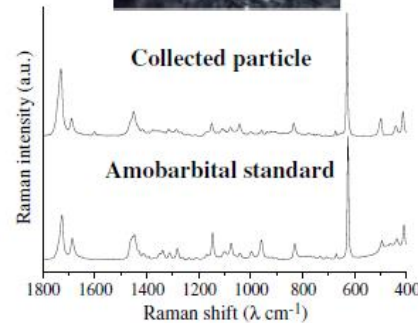
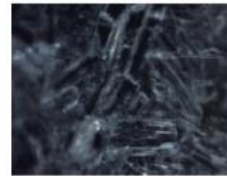
PARTICLE 1



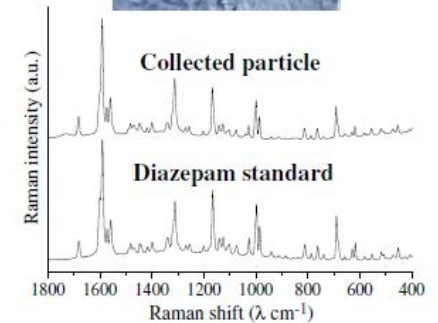
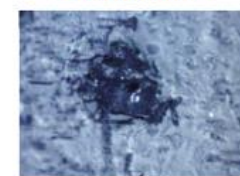
PARTICLE 2



PARTICLE 3

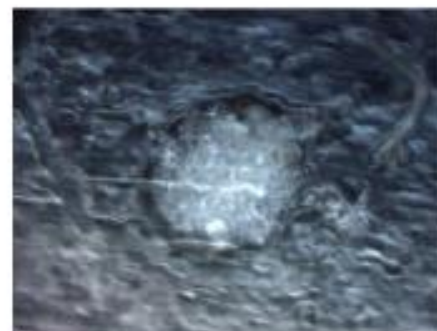


PARTICLE 4

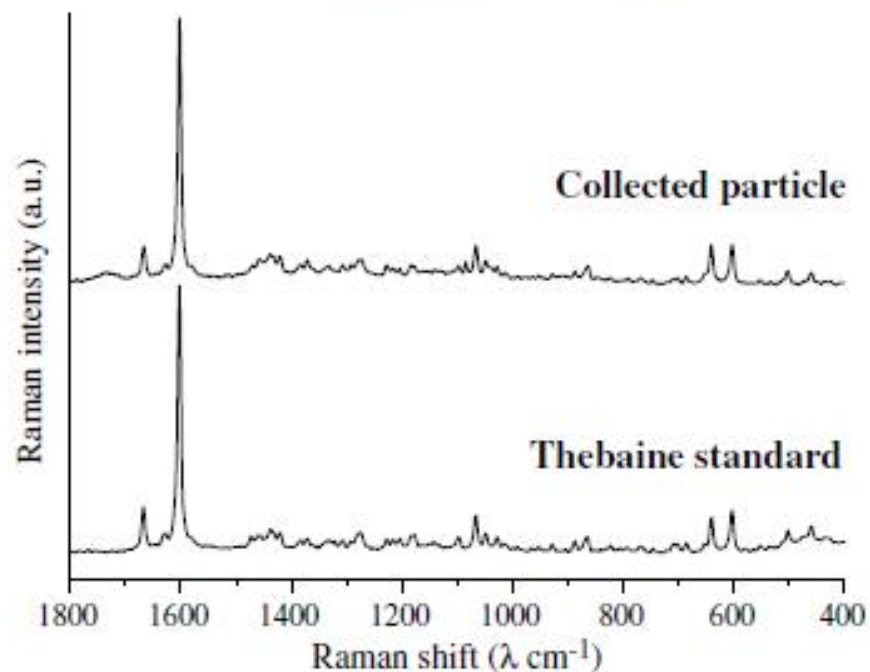


Substances Abuse Identification

Illicit drugs inside a pocket



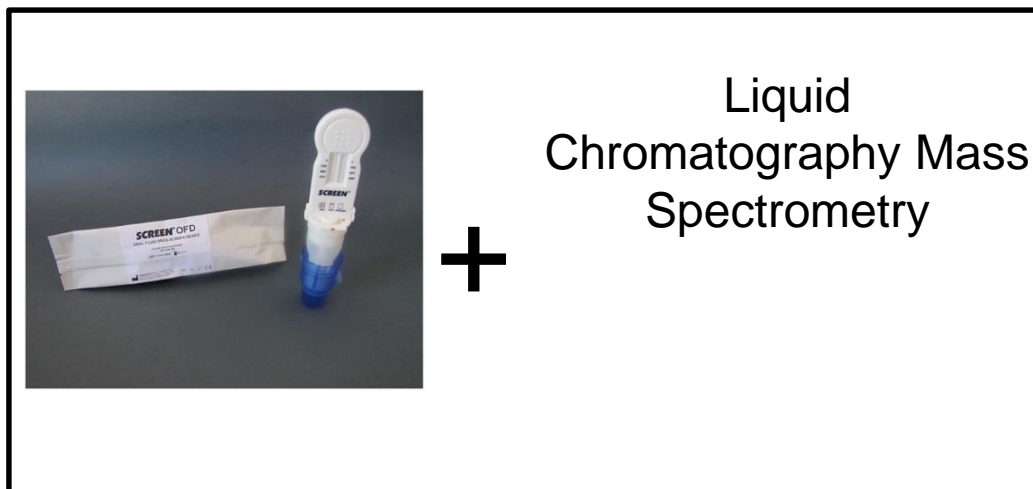
Magnification objective lens: 10×. Spectral acquisition times: 1 s × 50 acquisitions.
Laser power: 10.0 mW.



Substances Abuse Identification

SERS detection of illicit drugs for a future “in situ” detection device of drugs in oral fluid

Commercial immunoassay-based devices for presence analysis in oral fluids “in situ”



SCREEN OFD

+

Liquid Chromatography Mass Spectrometry



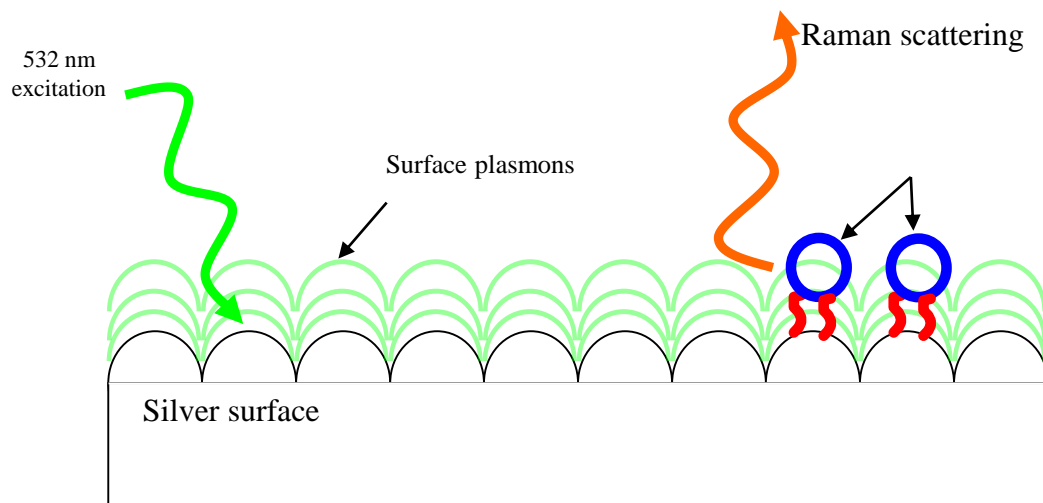
+

SERS

Presumptive test + Confirmatory analysis

SERS – What is it?

- Surface Enhanced Raman Spectroscopy
- Field enhancement of Raman scatter through interaction with a surface
 - Analytes on a metal surface, typically Ag or Au (can be vice versa with nanoparticles)
 - Electromagnetic field frequency in resonance with laser frequency
 - Signal enhancements up to 10^{14} have been reported
- Enables Raman analysis of extremely small or low concentration samples



SERS – What is it?

- Several different mechanisms contribute to SERS:
 - Generally classified as **electromagnetic and chemical effects**.
- **Electromagnetic effects** are a result of the increased electrical field strength caused by the interaction of the metal surface with light.
 - 1) **Concentration of electromagnetic field lines** at edges of metal particles (lightning rod effect),
 - 2) **Excitation of surface plasmons**. Surface plasmons are oscillations of conductance band electrons at the metal surface. At the surface plasmon resonance frequency, conductance band electrons move easily producing a large oscillation in the local electric field intensity. This surface plasmon resonance frequency depends on both the electronic structure of the metal and the size of the metal surface features (surface roughness or colloid diameter) [1].
- **Chemical effects** are due to the overlap of the analyte and metal wavefunctions.
 - They have a shorter range than the electronic effects and depend strongly on the identity of the analyte. Electromagnetic effects decrease as the cube of the distance from the metal surface. This can be several nanometers and, unlike chemical effects, is independent of analyte identity [1].
- **Important point**: The interaction of the sample with colloidal surface plasmons can lead to a quenching of any fluorescence. This enables good quality Raman spectra to be obtained from dye molecules

SERS for ink analysis

Application
Note: 52044

Determining Modifications to a Simulated Manuscript Using Surface-Enhanced Raman Scattering (SERS)

Timothy O. Deschaines, Ph.D., Thermo Fisher Scientific, Madison, WI, USA

Crow quill Pen



3 different black inks were used in this study:

2 iron gall inks (commercially available)- Ink made by tannic acid and iron salts (standard ink from the 5th to 19th century

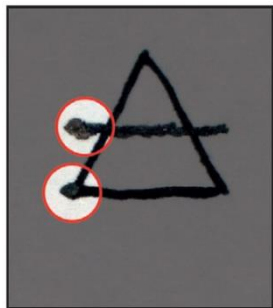
1 India ink

“original” figures → Alchemical Fire symbol made with 1 of the Iron gall inks

Horizontal line on the air symbol made with the Indian Ink

Plus sign on the sulfur symbol made with the 2nd Iron gall inks

SERS for ink analysis

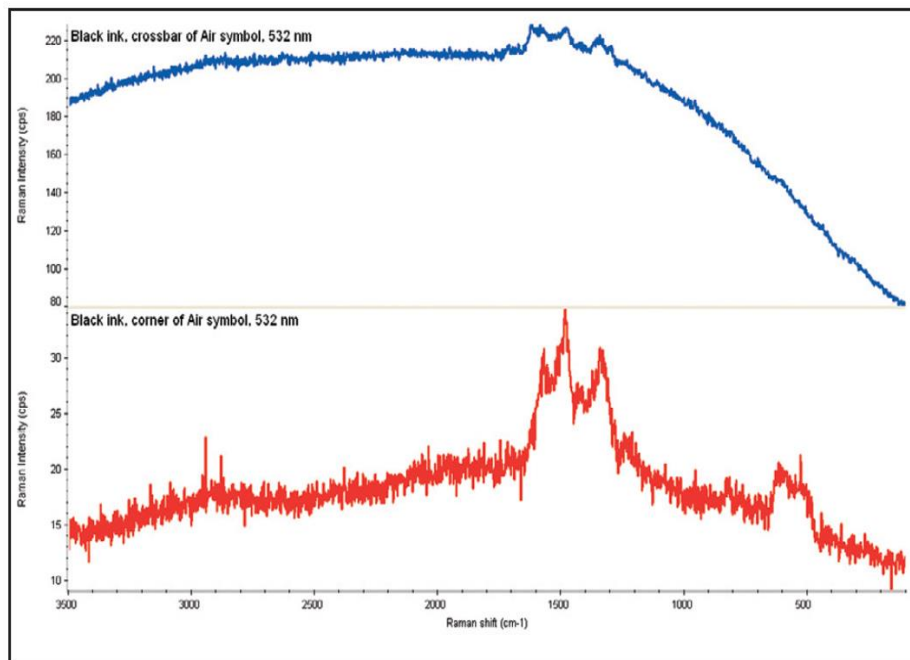


0.1 to 0.2 microliters of silver colloid were spotted on the two parts of the symbol

Application Note: 52044

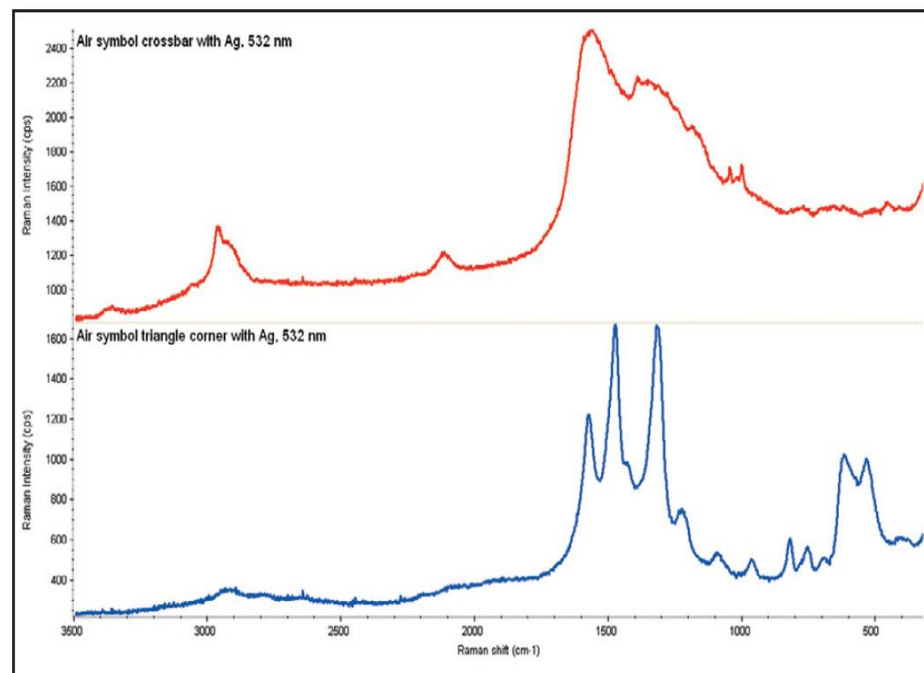
Determining Modifications to a Simulated Manuscript Using Surface-Enhanced Raman Scattering (SERS)

Timothy O. Deschânes, Ph.D., Thermo Fisher Scientific, Madison, WI, USA



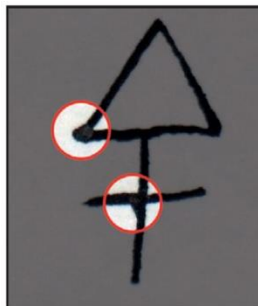
Before

After



SERS for ink analysis

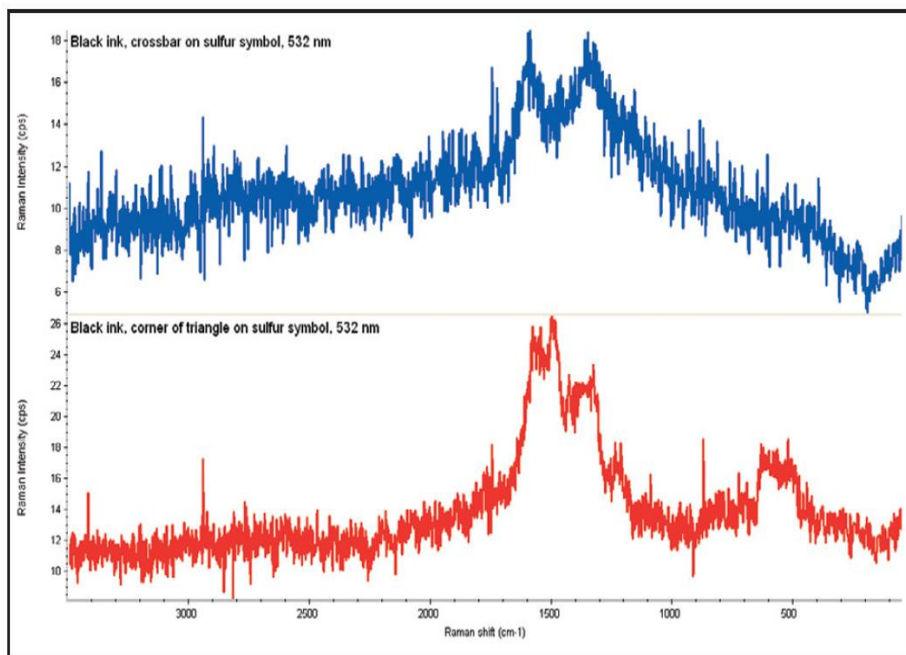
0.1 to 0.2
microliters of silver
colloid were spotted
on the two parts of
the symbol



Application
Note: 52044

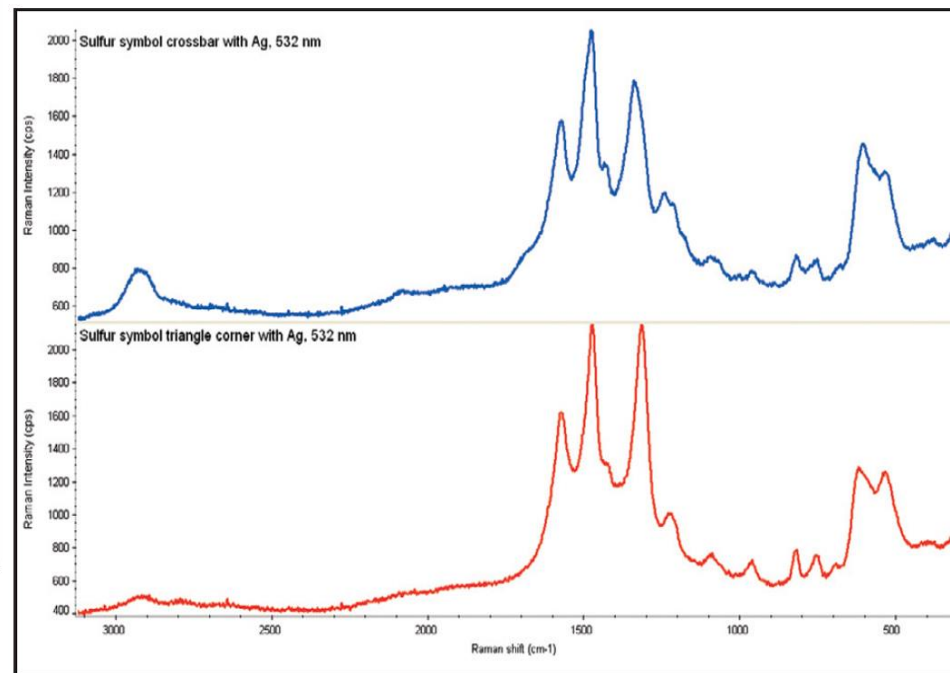
Determining Modifications to a Simulated
Manuscript Using Surface-Enhanced Raman
Scattering (SERS)

Timothy O. Deschânes, Ph.D., Thermo Fisher Scientific, Madison, WI, USA



Before

After

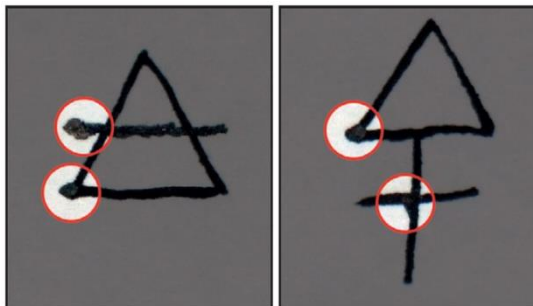


SERS for ink analysis

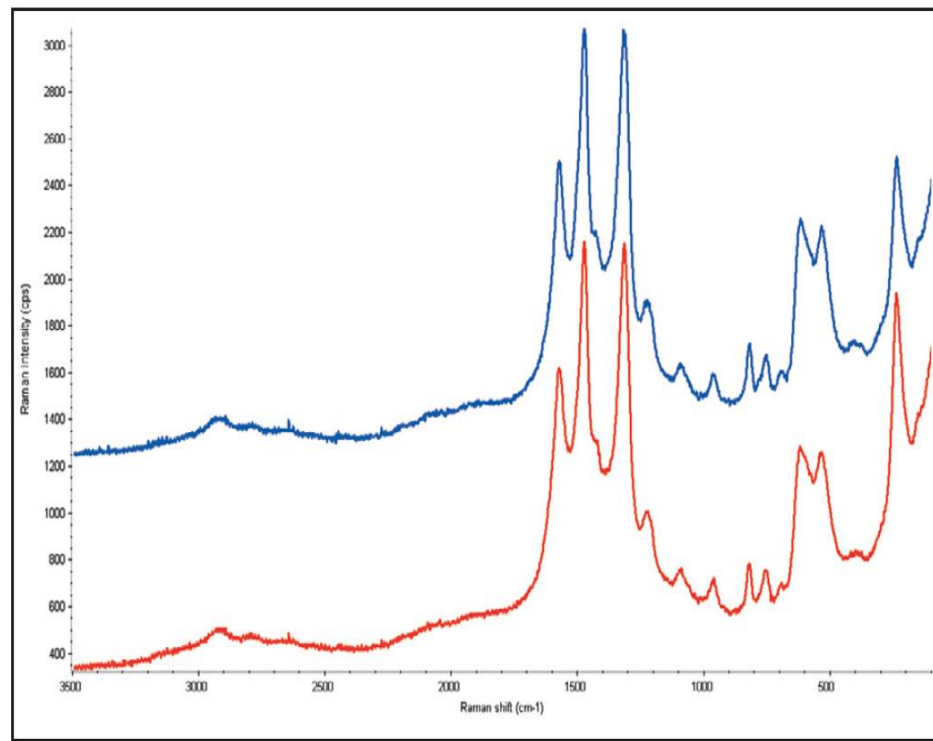
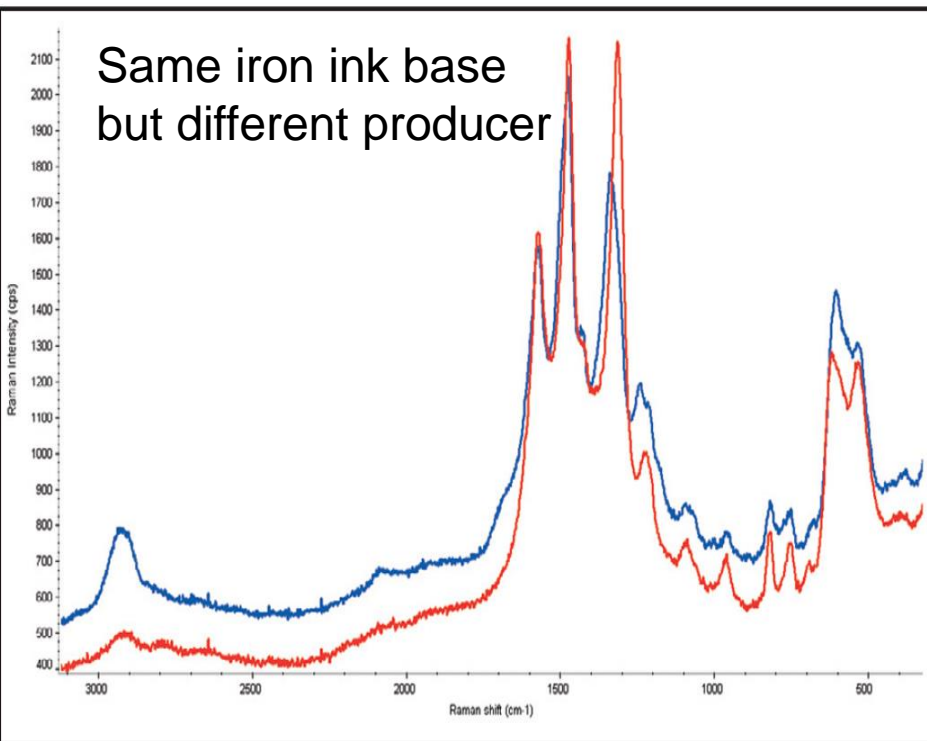
Application
Note: 52044

Determining Modifications to a Simulated
Manuscript Using Surface-Enhanced Raman
Scattering (SERS)

Timothy O. Deschânes, Ph.D., Thermo Fisher Scientific, Madison, WI, USA



Same iron ink base
but different producer

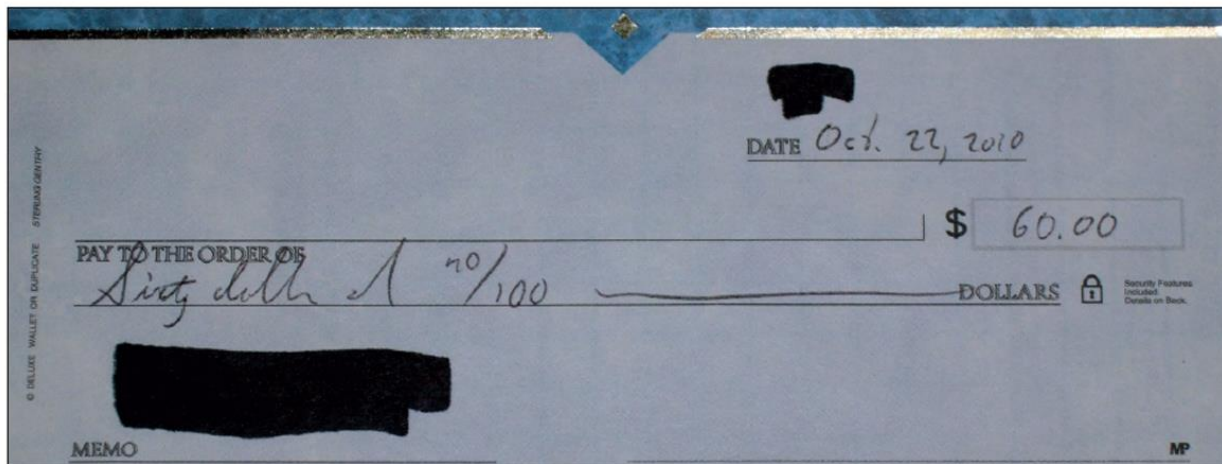


SERS for forged check

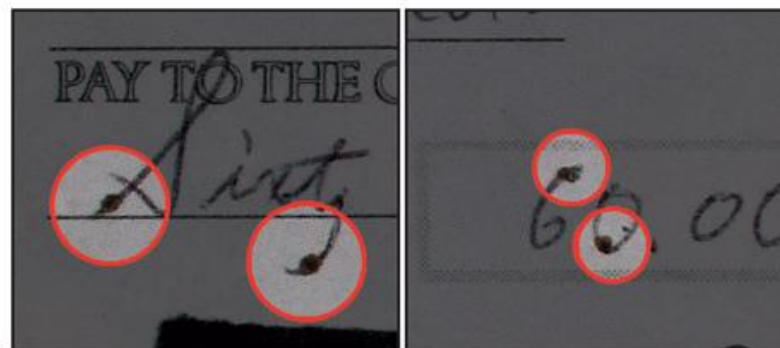
Application
Note: 52048

Analysis of Ink on a Forged Check Using
Surface-Enhanced Raman Scattering (SERS)

Timothy O. Deschaines, Ph.D., Thermo Fisher Scientific, Madison, WI, USA



Forged check – It was 6 dollars and we add a 0 and ...ty on
the check

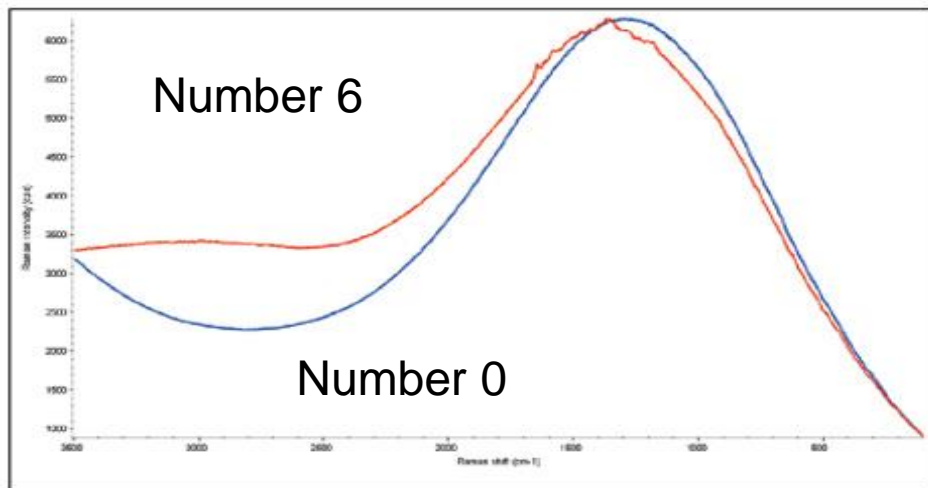
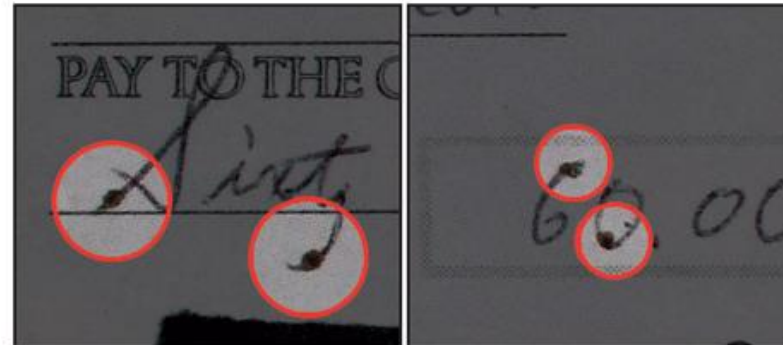
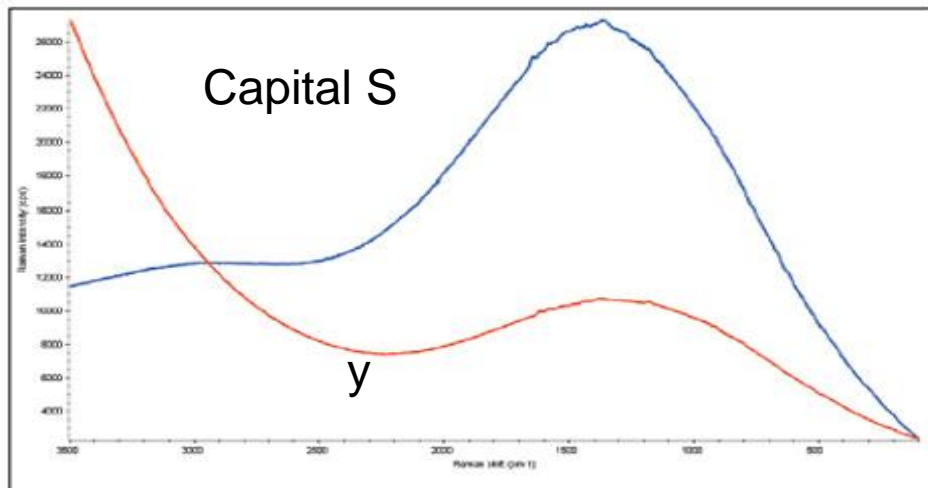


SERS for forged check

Application
Note: 52048

Analysis of Ink on a Forged Check Using
Surface-Enhanced Raman Scattering (SERS)

Timothy O. Deschaines, Ph.D., Thermo Fisher Scientific, Madison, WI, USA

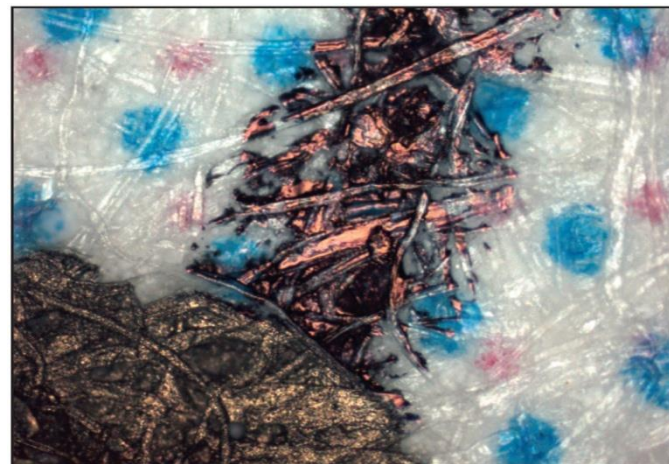
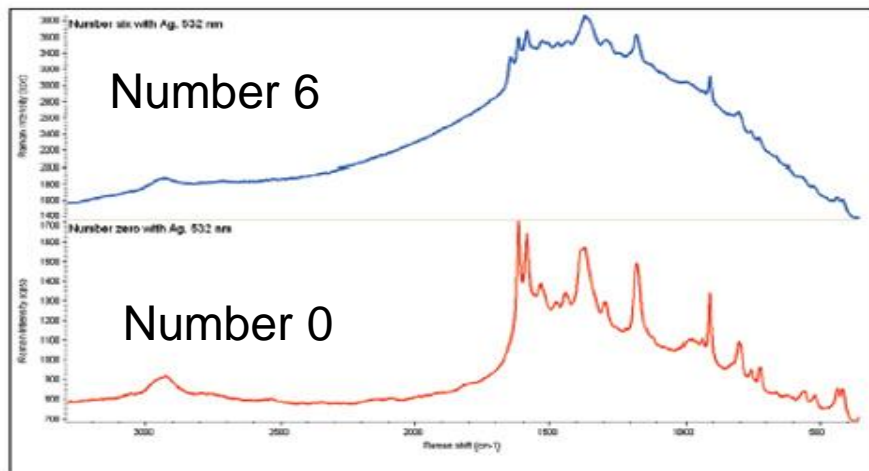
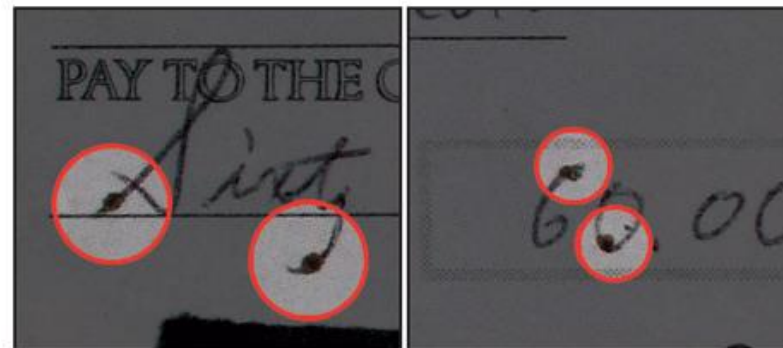
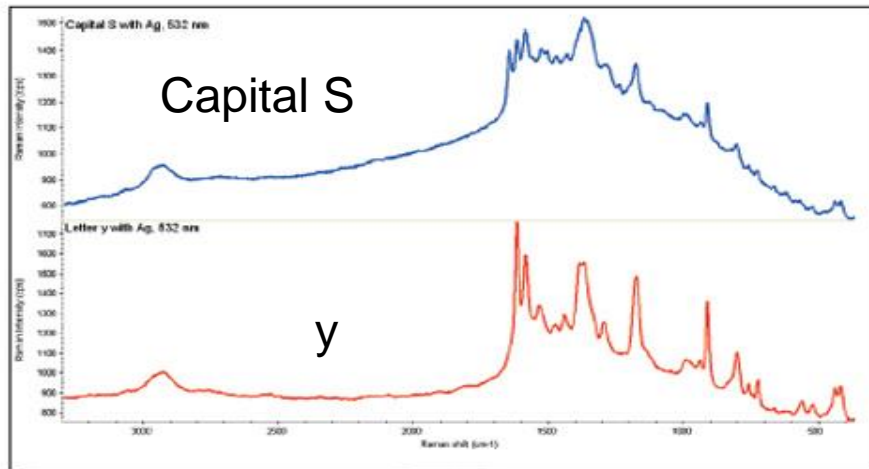


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Thank you!