

TechTIPS

Timely, Informative Productivity Solutions to Help You Work Smarter!

Mass Spectrometry

Molecular Spectroscopy

Elemental Analysis

Chromatography



Bring a friend!
Attend any LTQ
course (XL or
Orbitrap XL) and
receive 25%
OFF the second
enrollment.

TechTIP (LTQ Orbitrap XL™ Operations): Generating High Mass Accuracy Ion Lists

Picture this . . . You're setting up a data-dependent method on your LTQ Orbitrap XL and you find yourself unable to define your *parent mass* or *reject mass* list(s) with high mass accuracy.

What to do . . . In order to alter *Mass Lists* in the instrument setup of the LTQ Orbitrap XL and allow the input of masses with the low ppm mass accuracy, simply perform an external instrument calibration.

Here's how:

1. Open the *Instrument Configuration* icon on your desktop.
2. Select *Configured Devices – LTQ Orbitrap XL – Configure*.
3. Now, under *Display* in the LTQ Orbitrap XL configuration, change the mass precision of the mass lists to 5 ppm.
4. Once you've made the change (and this is important), restart Xcalibur™ and LTQTune.

Learn more when you attend:

LTQ Orbitrap XL Operations

Turn to Page 6 for Upcoming Course Dates!

Intended for users who are new to the Orbitrap system, this course covers the fundamentals of mass spectrometry, with emphasis on small molecule accurate mass applications. Users gain hands-on experience using both ESI and APCI ionization techniques and learn the benefits of accurate mass detection.

Topics include:

- Ion trap theory
- Orbitrap theory
- Tuning and calibration
- Hands-on APCI and ESI MS
- Instrument method development for LC/FTMS
- Multi-stage MSⁿ method building
- Parallel detection methods
- Accurate mass methods
- XCalibur software
- Basic LTQ maintenance

Browse courses or pre-register at www.thermo.com/education

TechTIP (For LTQ XL™ Operations): How to Get Rich. (Information-Rich Spectrum, That Is.)

A new dissociation technique called *Pulsed Q Collision Induced Dissociation* (PQD) allows you to obtain lower *m/z* fragment ions. PQD generates spectra qualitatively similar to CID, but in addition, allows the observation of low *m/z* fragments that are usually excluded from CID spectra because of the "one-third cut-off rule".

How PQD works:

1. Using a short-burst, high-amplitude resonance excitation pulse, the precursor ion is activated at a high Q value of "0.7".
2. Next, the ions are held at the high Q value for a short period of time – just long enough for the kinetic energy of the ions to be converted into internal energy through collisions, but NOT too long that significant dissociation would occur.
3. Finally, the precursor ions' Q value is pulsed to a low value by rapidly dropping the RF amplitude, and then allowing the precursor ions to undergo fragmentation at this low Q value.

This combination of activating at high Q values (high energies) and collecting fragments at low Q values (to trap low *m/z* fragments) results in an information-rich mass spectrum.

Learn more when you attend:

LTQ XL Operations

Turn to Page 6 for Upcoming Course Dates!

The LTQ XL Operations course is designed for users new to the LTQ XL mass spectrometer and covers mass spectrometry and chromatography in general, with emphasis on small molecule applications. Course includes lecture material, software training in addition to intense hands-on sessions that involve tuning, calibration, and comprehensive LC/MS method development using both electrospray and atmospheric pressure chemical ionization. A detailed training manual and a CD containing all data acquired during the training course are included, along with additional course materials.

Topics include:

- Ion trap theory
- Tuning and calibration
- Hands-on APCI and ESI MS
- Instrument method development for LC/MS
- Multi-stage MSⁿ method building
- Quantitative analysis
- Xcalibur software
- Basic LTQ XL maintenance

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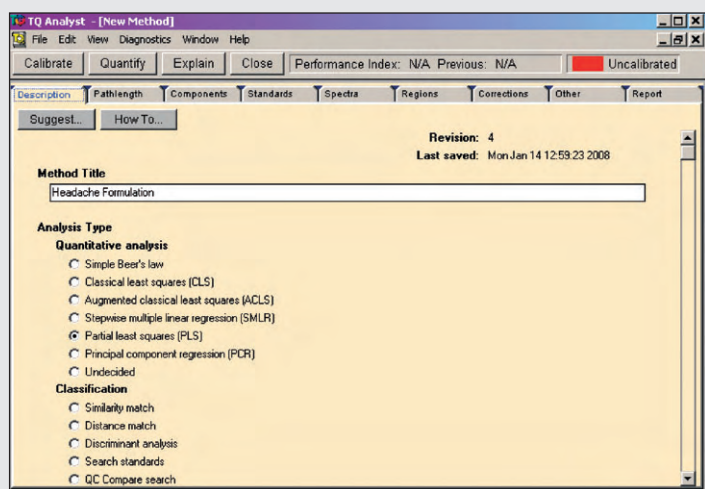


TechTIP (For TQ Analyst™ Software – Quantitative Operations): Developing the Best Calibration Model

As interest in quantitative infrared analyses continues to grow, the use of specialized calibration software is also on the rise. To accommodate the demand, *TQ Analyst* offers many advantages that go beyond what “generic” modeling packages provide, the software now pays much more attention to how *you* use it and how *you* set up your analysis to accommodate multiple users.

As one customer comments, “We needed a powerful, yet easy-to-use calibration package that didn’t require me to go back to college for additional advanced math or statistics courses, or cause us to sacrifice any of the flexibility to use it with a wide variety of applications.”

Bringing a host of integrated tools to the operator, *TQ Analyst* software allows both newly initiated and advanced users to perform functions to get the job done, in addition to being certain that the models they created will perform (as expected) in the real world.

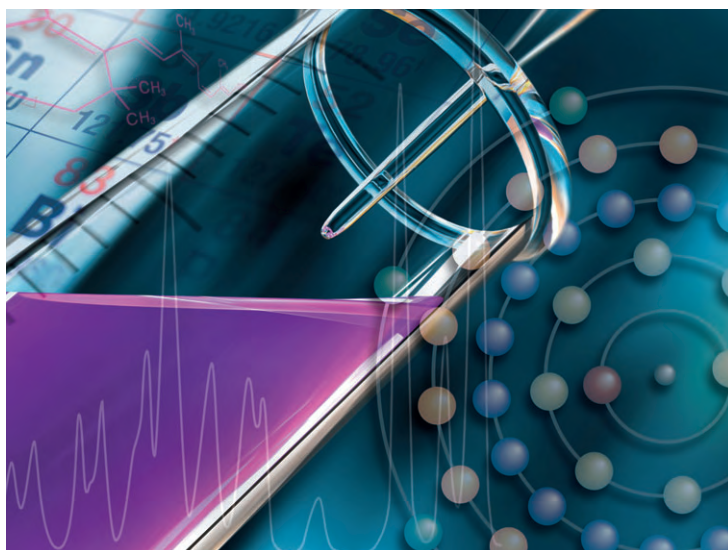


The *Help* menu also lets you choose an array of available example methods. You can even take a functions tour, where the software takes you through each step of the calibration process, allowing both newcomers and chemometric specialists alike, the analysis needed to construct the appropriate method.

Once the method has been created, *TQ Analyst* allows users choose from a number of very powerful post-calibration diagnostic tools, so they can evaluate the model, having the information necessary to decide where more improvements can be made.

In more complex methods, such as “Partial Least Squares Analysis”, factors are used to address the variability in the model. This means that when you calibrate a PLS method, the software will condense all of the relevant concentration and spectral information within the analysis region(s) of the calibration standards into a set of factors. (Each factor represents an independent source of variation in the data.) Factors are next ranked by the amount of variance they describe. (e.g., The first factor describes most of the variation in the calibration standards and each additional factor describes most of the remaining variation.) Accordingly, the first factor will contain most of the common information in the data. The rest of the factors contain information that is more specific, representing small variations in the data which are often important to the analysis.

The information provided by the *Factor Loading* diagnostic can help you identify standards that may be outliers, so you can decide whether or not to include them in your method.



Want to know more? Then don't miss this course . . .

TQ Analyst Quantitative Operations

Turn to Page 6 for Upcoming Course Dates!

2.0 CEU credits available

This course is designed for people who use vibrational spectroscopy to perform quantitative analysis. The course employs *TQ Analyst* for a variety of approaches to quantitative analysis including:

- Beer's law, classical least squares and partial least squares
- Classification analysis
- Quantitative method diagnostics
- Software wizards for feasibility and method performance

Prerequisites: Students are encouraged to bring data sets of spectra from analytical approaches they wish to create, but will be provided with an array of sample sets that will enhance their understanding of the material.

Browse courses or pre-register at www.thermo.com/education



Register for any Molecular Spectroscopy course before April 15 and receive 10% OFF the standard course price. (Promotion ends July 31, 2008)

TechTIP (For FT-Raman Spectroscopy Operations): Optimize Tuning between Infrared and Raman Analysis

When switching between infrared and Raman analysis on your FT-Raman system, it is necessary to fine tune the system alignment. One of the easiest ways to accomplish this (and ensure that you have the best possible throughput prior to beginning your analysis) is to use the white light, in addition to a small amount of KBr powder in the NMR tube.

To switch between infrared and Raman analysis modes, it becomes necessary to change the beamsplitter on instruments where both a KBr and CaF₂ beamsplitter are available. Here's how:

1. The first step of this process should be to change splitters while still in the FT-IR mode and perform the align function in the *Collect | Experiment Setup | Diagnostics* tab(s).
2. Next, choose Use *Raman Accessory* in the Raman menu and find the focal point of the optics by observing where the He:Ne laser focuses. (To do this, place an index card in the beam path of He:Ne beam. Move the index card along the beam axis and note where the small laser spots are most tightly focused. This will be the proper position for your sample.)
3. Now adjust the sampling accessory to this approximate location through *Experiment setup/Bench* window under Raman Accessory Control (see Figure 1).
4. Place an NMR tube – filled with KBr powder in the accessory – and turn the white light up to medium in the *Raman Source* setting area. **You should now see an FT-Raman interferogram in the real-time interferogram window.**
5. You may now manually adjust the focus until you see the Peak-to-Peak intensity reach a maximum or alternatively choose the autofocus option to have the software find the optimal position for you.

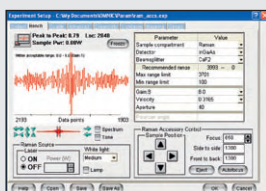


Figure 1

Now that the NMR tube placement is optimized in the bench, all you have to do is to go to *Diagnostics* tab (see Figure 2) and click on align. Your FT-Raman system is now optimized.



Figure 2

Learn more when you attend:

FT-Raman Spectroscopy Operations

Turn to Page 6 for Upcoming Course Dates!
2.0 CEU credits available

This course is designed for students who wish to explore the best of FT-Raman spectroscopy. Using a blend of discussions, hands-on demonstrations and student activities, this course highlights array automation and micro Raman spectroscopy and will also cover:

- Optimizing software parameters
- Quantitative and qualitative analysis
- Implementing spectrometer validation
- Sample preparation approaches for improved spectral quality
- Automating sample collection using the MicroStage/ViewStage accessory

Note: This course does not cover dispersive Raman instruments. Please refer to the Nicolet™ Almega™ XR Operations course.

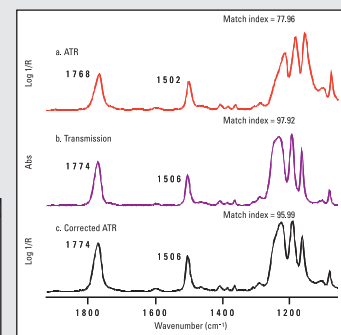
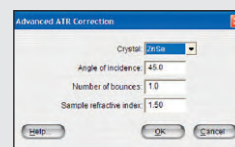
TechTIP (For Fundamentals of FT-IR Microscopy Operations): The Benefits of Micro-ATR

Micro-ATR allows one to analyze samples embedded in a matrix without the need for extraction, compression or any other sample preparation that can delay the process.

Place the sample on an aluminum or gold coated mirror and insert this into the contact alert plate holder (Ensure that the contact alert plate is plugged in to the instrument). Then, place the sample under the objective and focus on the area of interest. Next, slide the ATR tip into position (you may need to lower the stage for this) until you hear a “click”. Turn on the preview function in *Experiment Setup* to monitor the spectral response as you gradually bring the sample into contact with the ATR. As the sample comes into intimate contact with the ATR, peaks will begin to appear in the spectrum. The background in any ATR experiment is a spectrum acquired with a clean crystal in air.

ATR spectra are NOT identical to transmission spectra because the technique distorts spectral features. However, it is possible to correct for this distortion (if you use OMNIC™ software) by simply applying the *advanced ATR correction option* (Note: reference spectra in commercial libraries will appear in ‘transmission format’ unless otherwise specified).

The figures below show the effect of ATR correction on the *search match values* of a polycarbonate sample spectrum. The uncorrected ATR spectrum yields a match value that is 20% lower than the transmittance data. However, once the ATR correction is applied, the match value is significantly increased and is close to the transmittance value.



a. ATR spectrum of polycarbonate Match index = 77.96

b. Transmission spectrum of polycarbonate thin film. Match index = 97.92

c. Advanced ATR correction applied to spectrum (a). Match index = 95.99

Learn more when you attend:

Fundamentals of FT-IR Microscopy Operations

Turn to Page 6 for Upcoming Course Dates!
3.0 CEU credits available

Employing a unique combination of software training with instrumental demonstrations and hands-on activities, students will gain practical experience related to effective sample preparation and data acquisition. Topics include:

- OMNIC FT-IR software operations
- Microscope operation and performance verification
- Sample preparations for reflection microscopy including attenuated total reflectance
- Sample preparations for transmission microscopy
- Spectral interpretation introduction

Software and microscope operations training vouchers may be used as partial payment for this course.

TechTIP (For ARL OES Operations):**Precision vs. Accuracy: How They Impact Your Results**

Do you know the parameters which are most important to controlling your OES instrument so that it provides consistently correct results?

The analytical precision achievable on your instrument is directly influenced by many variables that must be under control and these along with instrument calibration can affect whether the results on samples are consistently correct or not.

One such variable is the quality of argon gas being used. If the level of oxygen as a contaminant in the argon is too high, it will result in a bad burn causing poor precision.

Another important consideration would be the characteristics of the calibration. That is, "Are the standards I'm employing truly representative of the material I'm analyzing?"

Learn about this topic and more when you attend . . .

ARL OES Operations

Turn to Page 6 for Upcoming Course Dates!

This four day course is designed for the user who is new to the ARL MA, 2460, 3460, and 4460 spark emission instruments accompanied WinOE software. New users will learn the skills necessary to operate the instrument and optimize results for their specific applications. The course is divided into lecture and hands-on laboratory time to gain a working knowledge quickly.

Topics include:

- Spark emission theory
- Hardware and software overview
- How optimize results
- Precision and accuracy improvement
- Calibration
- Matrix Dilution
- Inter-element corrections
- Drift Correction
- Type standardization
- Sample Preparation
- Trouble shooting analytical data
- Routine Maintenance
- And more!

Browse courses or pre-register at www.thermo.com/education

**Bring a Friend!**

Attend Atomic Absorption Operations at the standard price of enrollment, and **receive 20% OFF** the second enrollment.

(Offer valid thru 12/31/2008. Participant(s) need not attend the same course date for offer to be valid.)

**TechTIP (For Atomic Absorption Operations):****How to View Concentration Readings in Real Time**

In the spectrometer status window, one typically sees the absorbance displayed in real time. This absorbance display is useful for flame work and is particularly useful for optimizing the burner head position.

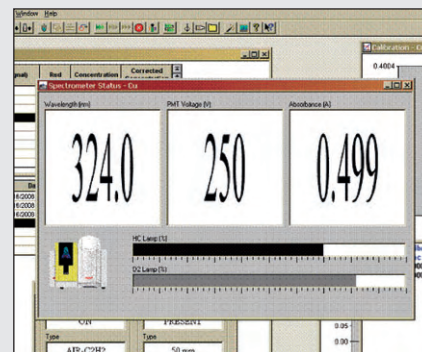


Figure 1: The default view of the "Spectrometer Status window" indicating absorbance

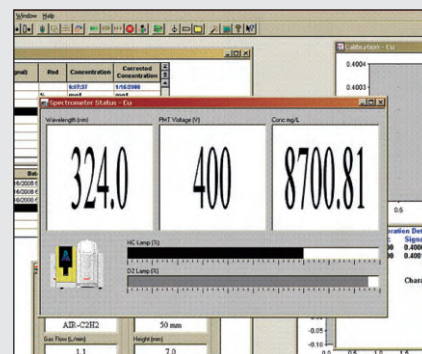


Figure 2: You can also switch the absorbance display to concentration display by simply right-clicking on the display window and selecting *Display Concentration*. By doing this, you can quickly aspirate samples and view concentration readings.

Learn more when you attend . . .

Atomic Absorption (AA) Operations

Turn to Page 6 for Upcoming Course Dates!

Presented in a lecture/lab format, this course covers all essential topics regarding flame/furnace optimization, methods development and efficient operation of the instrument. Both *D2* and *Zeeman* background correction techniques will be explored.

Topics include:

- Atomic spectroscopy theory
- Solaar™ Atomic Absorption software
- Instrument optimization
- Methods development
- Troubleshooting

Note: Flame and furnace AA users will partake in a four-day course. Flame ONLY users will attend the first two days of this course at 50% off the cost of standard enrollment.

Browse courses or pre-register at www.thermo.com/education

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Bring a Friend!

Attend DSQ/DSQ II (with TRACE GC Ultra) Operations at the standard price of enrollment, and **receive 20% OFF** the second enrollment.

(Offer valid thru 12/31/2008.

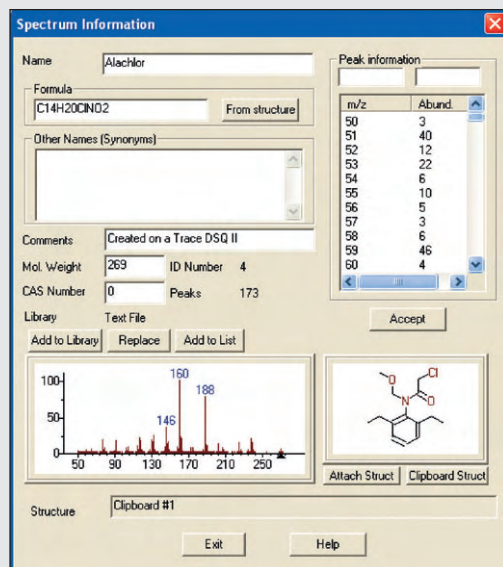
Participant(s) need not attend the same course date for offer to be valid.)

TechTIP (For DSQ™/DSQ II™ with TRACE GC Ultra™ Operations): Creating Your Own Unique User Library

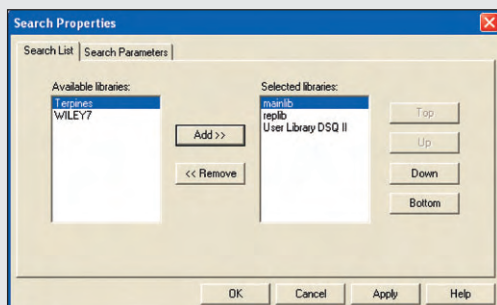
One of the best features of a GC/MS is the generation of spectra that can be searched against commercially available libraries. This is possible, because most GC/MS users now follow the same protocols for calibrating and obtaining spectra.

Examples of those protocols include the use of PFTBA as a mass spectrometer calibrant, as well as the use of 70 eV ionization filament energy. Since commercial libraries use spectra from different types of mass spectrometers (i.e., Quadrupoles, Magnetic Sectors, TOF, Ion traps), slight variations will appear in the spectra that is obtained. For this reason, it is a good idea to generate spectra related to a particular instrument, and then save that particular spectra as a library for unknown identification.

The TRACE DSQ II with Xcalibur software has the ability to take generated spectra and create a user library that uses the NIST format. This type of spectra can then be used in conjunction with that particular instrument for sample processing and peak identification. The figures below show this process.



Once the information for a particular component has been entered, all you need to do is save it to a user defined library by doing this:



User libraries will result in better library search matches which means better certainty in unknown identification.

Learn more when you attend:

DSQ/DSQ II (with TRACE GC Ultra) Operations

Turn to Page 6 for Upcoming Course Dates!

Gain a complete understanding of the operation and maintenance of the TRACE GC Ultra oven and DSQ/DSQ II mass spectrometer, plus a working knowledge of Xcalibur software. Course consists of lectures in addition to laboratory experiments where participants will create qualitative and quantitative analysis, processing methods, and reports. Lectures and course notes will be provided for both instrument and software lessons.

Topics include:

- Set-up and maintenance of the DSQ/DSQ II, TRACE GC Ultra
- Set-up and maintenance of the AS3000 and TriPlus™ autosamplers
- Xcalibur processing methods (qualitative and quantitative analysis)
- Merlin reports
- User libraries
- Chemical ionization
- Probe analysis

Prerequisites: Students should have a general understanding of mass spectrometry, gas chromatography and Windows® software.

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Upcoming Seminars, Webinars and Events

- 2008 Winter Research Symposia (RSS), multiple dates and locations
- 2008 Spectroscopic Solutions (S3), multiple dates and locations
- 2008 Trace Elemental Seminars (TEA) Microanalysis Seminars, multiple dates and locations
- Near IR Webinar Series, multiple dates
- ConExpo/ConAgg, March 11-15, Las Vegas, NV
- ANTEC, May 4-8, Milwaukee WI, USA
- AISTech, May 5-8, Pittsburgh, PA
- SEMICON West, July 15-17, San Francisco, CA, USA
- The XVth International Congress on Rheology, August 3-8, California, USA

For more information on all our North American events and seminars visit:
www.thermo.com/naevents



2008 Course Schedule

COURSE TITLE	April	May	June
CHROMATOGRAPHY AND MASS SPECTROMETRY (WEST PALM BEACH, FL; SAN JOSE, CA; BOSTON, MA; KANSAS CITY, MO; LAS VEGAS, NV)			
LCQ™ Operations	28 → 1 FL		
LCQ Biotech Operations		5-8 FL	
LTQ XL™ Operations	7-10 FL	5-8 FL	2-5 FL
LTQ XL Biotech Operations		12-15 FL	
LTQ XL w/ETD Operations		19-22 FL	
LTQ XL OrbiTrap Operations		5-8 FL	9-12 FL
LTQ XL OrbiTrap Biotech Operations	14-17 FL		23-26 FL
LTQ XL FT/LTQ XL FT Ultra Operations	3 CA		
LTQ XL FT/LTQ XL FT Ultra Biotech Operations			
TSQ™ Quantum Operations	7-10 FL	12-15 FL	2-5 FL
QuickQUAN™ Software Operations		20-22 FL	
Surveyor MSQ Plus™ Operations	8-10 CA		10-12 CA
Polaris Q (with TRACE GC Ultra™) Operations		4-7 FL	10-13 FL
DSQ/DSQ II™ (with TRACE GC Ultra) Operations	21-24 FL		2-5 FL
ToxLab™ Software Operations		28-30 FL	
Basic HPLC Training			
HPLC Method Development for LC/MS Operations			
BioWorks™/SEQUENT™ Software Operations	24-25 CA		24-25 FL
Xcalibur™ Software Module	21-23 CA	28-30 FL	
ChromQuest™ Software Module – GC	1-3 FL		
ChromQuest™ Software Module – LC		20-22 FL	
Accela™ UHPLC Training			10-11 FL
Mass Frontier™ 5.0 Software Operations		15-16 CA	19-20 FL
MetWorks™ Software Operations		13-14 CA	17-18 FL
EI/CI Interpretation Module	8-9 FL		
Basic Gas Chromatography	15-16 FL		
Gas Chromatography Method Development	29 → 1 FL		
EnviroLab™ Forms 2.0 Software Operations			23-26 FL

COURSE TITLE	April	May	June
MICROANALYSIS (MADISON, WI)			
NORAN System SIX Operation			24-27 WI

COURSE TITLE	April	May	June
ELEMENTAL ANALYSIS (WEST PALM BEACH, FL; SCHAUMBURG, IL, MADISON, WI; DEARBORN, MI)			
XSERIES 2 ICP-MS Operations		6-9 FL	
iCAP 6000 Series Operations		20-23 FL	17-20 FL
Atomic Absorption Operations		13-16 FL	
IRIS Intrepid ICP Operations		*Onsite Training Course	
ARL QuantX EDXRF Operations	1-4 FL		
ARL XRF/XRD Operations	28 → 1 FL		16-19 FL
ARL OES Operations	8-11 FL		3-6 FL

COURSE TITLE	April	May	June
MOLECULAR SPECTROSCOPY COURSES (WEST PALM BEACH, FL; MADISON, WI; SAN FRANCISCO, CA; LAS VEGAS, NV)			
FT-IR Spectral Interpretation			9-13 WI
Fundamentals of FT-IR Analysis			2-6 WI
Fundamentals of FT-IR Microscopy Operations	21-25 WI		
Nicolet Antaris™ FT-NIR Analyzer Operations	8-10 IL		
Nicolet Centaurus™ Microscope Operations		13-15 WI	
Nicolet Continuum™ Microscope Operations		6-9 FL	17-20 FL
Nicolet ECO™ FT-IR Metrology Tool Applications			
TQ Analyst Software – Quantitative Operations			
Almega™ Raman Operations		6-8 WI	
FT Raman Spectroscopy Operations	29 → 1 WI		
FT-IR Gas Analysis Software			
OMNIC™ Software Essentials Operations	22-24 FL	20-22 FL	17-19 FL
OMNIC Software Plus Operations		6-9 WI	

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