

# TechTIPS

Timely, Informative Productivity Solutions to Help You Work Smarter!

Mass Spectrometry

Molecular Spectroscopy

Elemental Analysis

Chromatography



Receive a FREE 50 x 2.1 mm, 1.9  $\mu$ m, Hypersil GOLD™ Column when you attend the TSQ Quantum Operations or the LTQ Orbitrap Operations Course!

A \$600 dollar value!  
(P/N 25002-052130)

Use promotion code: 51394 when pre-registering.

Attention GC/MS Users

See our NEW EI/CI Interpretation Course in the Chromatography Section, inside!

## TechTIP: Achieve Better SRM Transitions

For reproducible quantitative SRM methods the chromatographic peak should be appropriately sampled. To increase the sampling efficiency of your SRM transitions, think about employing multiple segments and/or varying scan times for each transition – especially when developing methods with a large number of components.

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

### TSQ Quantum Operations

July 23-26, 2007 | August 27-30, 2007  
West Palm Beach, FL

This course will familiarize the TSQ Quantum™ user with basic instrument operation, including API and quadrupole theory, tuning, calibration, data collection, maintenance, and general functionality of the Xcalibur™ software package. The course will be presented in a lecture/workshop format where the students will have an opportunity to interpret data and present their findings to the class.

#### Topics include:

- Development of the TSQ Quantum
- Fundamentals of mass spectrometry
- Ion Max Source
- TSQ Quantum hardware
- TSQ Quantum scan modes
- TSQ Quantum instrument control
- Xcalibur, XReport™, LCQUAN™
- User maintenance

*Prerequisites:* Understanding of the principles of organic chemistry, as well as basic chromatographic skills.

Pre-register at [www.thermo.com/education](http://www.thermo.com/education)

## TechTIP: LTQ Orbitrap – Obtain Specific Extracted Ion Chromatograms

After acquiring high resolution data using the LTQ Orbitrap, an extracted ion chromatogram can be generated using a narrow mass tolerance. Xcalibur™ software uses the tolerance value to create limits for a specified mass range. For an extracted ion chromatogram, simply type in the exact mass of an ion to be extracted – specifying a mass tolerance value of 5 ppm or less for the mass tolerance value. The chromatogram generated will be more specific to your ion of interest than an extracted ion chromatogram that uses the default mass tolerance value of 500 mpp.

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

### LTQ Orbitrap Operations

July 30-August 2, 2007 | September 24-27, 2007  
West Palm Beach, FL

The LTQ Orbitrap™ Operations course provides general overview of chromatography and mass spectrometry, with an emphasis on small molecule, accurate mass applications. The course includes lectures, software training and hands-on sessions involving tuning, calibration and comprehensive LC/FTMS method development using both electrospray and atmospheric pressure chemical ionization techniques. Instrument method development will focus both on accurate mass determination of small molecules and fragments and parallel detection methods. A detailed training manual and a CD containing data acquired during the course are included, along with other course materials.

#### Topics include:

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

*Prerequisite:* Practical LC/MS for Beginners course or previous experience developing LC/MS methods. (Experience in FTMS is not required).

Pre-register at [www.thermo.com/education](http://www.thermo.com/education)

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A \$600 dollar value! (P/N 25002-052130)

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## COMING SOON!

### Productivity Solutions Training

- EPA 8260 (Volatiles)
- 525 (Semi-Volatiles)
- 524 (Volatiles)

To inquire, visit:  
[www.thermo.com/education](http://www.thermo.com/education) and click 'Contact a Training Representative'

## Congratulations, Sung Jung!

### Winner of the Training Course Sweepstakes

*Proteomics Core Manager  
Baylor College of Medicine  
Houston, TX*



Sung Jung with his Thermo Scientific LTQ Ion Trap Mass Spectrometer

**TechTIP: IR Spectral Interpretation**

Spectral interpretation is a honed skill. Molecular ID can be performed through first identifying functional groups in the higher frequency range. Then, molecular structure can be realized from fine spectral features found in the fingerprint region – all assisted by digital libraries and interpretation tools recently made more available.

**Example:** The symmetric and asymmetric methyl stretching modes are observed at 2930 and 2850  $\text{cm}^{-1}$ , respectively. The presence of the methyl group is further confirmed by the presence of the symmetric deformation mode at 1375  $\text{cm}^{-1}$ . When this symmetric deformation mode is split into a doublet in equal intensities, geminal-dimethyl or isopropyl special branching structure can be realized.

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

**FT-IR Spectral Interpretation**

July 24-27 | Madison, Wisconsin | 2.6 CEU credits available

This course provides an extensive review of the interpretation of mid-infrared spectra, and will show students how to interpret FT-IR spectra for structural information. Presented in a lecture/lab format, students will have the opportunity to interpret data and present their findings to the class. Students are encouraged to bring spectra from their laboratory to discuss with the class.

**Classifications to be covered:**

- Alkanes and branched alkanes
- Aromatics
- Ethers and alcohols
- Halides
- Sulfurs, phosphorus, silicon and boron compounds
- Alkenes and alkynes
- Carbon containing alkyl groups
- Amines, amides, and nitro compounds
- Inorganics
- Interpretive aids

*Prerequisite:* Understanding of the principles of organic chemistry.

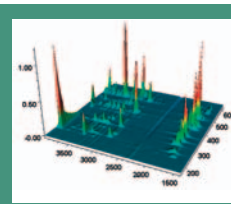
**FT-IR instrument software training vouchers may be used as partial payment for this course.**

Pre-register at [www.thermo.com/education](http://www.thermo.com/education)

**TechTIP: Get to Know TQ Analyst**

TQ Analyst™ software is a powerful multi-variant modeling package, primarily used to create calibration models for infrared spectral features. In addition to this use, the tools available in the software can be used to solve many problems without having to create calibration models.

**Problem Solved:** A tungsten layer was being deposited on top of various silicon dioxide layers. The tungsten films were exhibiting “holes”, which lead to failures in the final product. Spectra were collected from the oxide films and simple counts of the holes in the tungsten layers were made. After transferring all this information into the TQ Analyst software (and using the diagnostic tools), results showed a correlation of the O-H stretching in the oxide films to the number of holes in the tungsten layer. Because silicon dioxide can have surface -OH functional groups that can attract moisture to the surface, a simple bake of the material removes this -OH group prior to the deposition of the tungsten layers, solving this problem.



Upgrade to OMNIC™ 7.3 today and collect data faster, easier! Includes many NEW features, PLUS 7 bonus features to give you the best value for your lab!

**A \$5,500 value, yours for only \$1,500!\***

To learn more visit [www.thermo.com/omnic73](http://www.thermo.com/omnic73).

(\*Analytical OMNIC 7.3 upgrade package.)

**TQ Analyst Software NOW INCLUDED with certain variations of OMNIC software!**

Call 800-437-3847 for details.

Get a **FREE Multi-Element Lamp** when you attend the AA Operations course!

- Ca/Mg/Si (P/N 942339321061)
- Al/Si/Ti (P/N 942339321391)
- Co/Cu/Mn/Fe (P/N 942339321331)

**A \$500+ Value, Your's FREE!**

Use promotion code: 51394 when pre-registering.

**TechTIP: Atomic Absorption (AA) – Get the Acetylene Out!**

When you finish running your flame analysis, you naturally shut the flame down and then turn off the acetylene at the cylinder. *But how can you get the acetylene out of the supply lines?* Easy. Simply press and hold the red “Flame Off” button on the instrument. Within several seconds the acetylene will be bled from the supply line and the instrument. When you release the red button, any residual acetylene will be flushed out with air.

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

**Atomic Absorption (AA) Operations**

August 7-10, 2007 | West Palm Beach, FL

Presented in a lecture/lab format, this course covers all essential topics regarding flame/furnace optimization, method development and efficient operation of the instrument. Both  $\text{D}_2$  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 users will have a four-day course. Flame-ONLY users will attend the first two days of training at a cost of 50% of enrollment.

Pre-register at [www.thermo.com/education](http://www.thermo.com/education)

**TechTIP: WDXRF Operations – Change the Acquire Time Without Recalibrating**

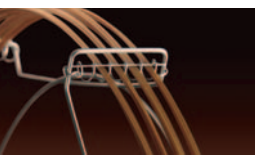
It is possible to change the acquire time in a calibrated *WinTrace Method* without having to recalibrate.

**For Speedy Acquisition:** If a high degree of precision is not necessary, save a copy of your calibrated method with a shorter acquire time – the calibration coefficients will still be valid. Using this approach, it is possible to have methods to preview, “screening” your samples quickly.

**Discussion of Precision for XRF Analysis:** The acquire time in a method affects the precision of measurements made with the method. The error in a measurement is related to the square root of the number of x-ray counts for the analyzed element. So, in order to improve the precision by a factor of two (that is, to cut the error in half), the acquire time must be increased by a factor of four (because of this square root term).

The relationship between acquire time and precision means that while you must acquire for much longer to improve precision, you won't pay as large a penalty in precision for decreasing the acquire time – cutting the time to one-quarter of the original value will only result in a doubling of the relative error.

Want to know more? Then don't miss **ARL XRF/XRD Operations . . .**



Receive a FREE GC Capillary Column when you attend ANY GC or GC/MS course!

Choose from the following:

- **TRACE-5MS Low-Polar Column** (P/N 260F142P)
- **TRACE-1701 Mid-Polarity Column** (P/N 260Q142P)
- **TRACE-Wax MS High-Polarity Column** (P/N 260X142P)

Use promotion code: 51394 when pre-registering.

### TechTIP: Interpret a Mass Spectrum— Even When it's Not in the Library

Mass spectra are part of the results generated by GC/MS when a sample is analyzed. When the sample contains compounds that are not in the library, identification can be performed by interpreting the mass spectra. This is possible because mass spectra are like a fingerprint of the compound.

Typically, the first thing you'll need to do is determine the molecular weight of the compound. In other words, find the molecular ion in the mass spectrum. There are some rules that a suspected molecular ion peak in the mass spectrum has to follow in order to be identified as the molecular ion.

Because Electron Ionization (EI) involves a large amount of energy, it may cause the molecule to fragment so much that the molecular ion doesn't survive.

There is another alternative, Chemical Ionization (CI). CI involves less energy than EI, producing less fragmentation and making the determination of the molecular weight of the compound easier. Once the molecular weight is determined using CI, interpretation of the fragmentation seen within the EI spectrum can be done. *NOTE: Different compounds are going to fragment differently, depending of their chemical structure.*

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

### Attention GC/MS Users

#### EI/CI Interpretation Module

July 31-August 2, 2007 | West Palm Beach, FL

This course is designed to introduce the underlying principles of classical mass spectrometry and teach the fundamental processes involved in interpreting electron ionization (EI) and chemical ionization (CI) mass spectra.

#### Topics covered:

- Electron ionization theory
- Chemical ionization theory
- The nitrogen rule
- The double bond equivalent formula
- Isotopes for interpretation purposes
- Fragmentation mechanisms
- Commercial and user libraries
- Computer tools for spectral interpretation

Pre-register at [www.thermo.com/education](http://www.thermo.com/education)

### TechTIP: Leaky GC Injector? Try This!

Use this procedure if you suspect a leak in your GC injector or carrier gas plumbing lines.

#### Finding the Leak(s):

1. Remove the column from the injector and plug the column connection so there is no flow coming out of the bottom of the injector. (Most GC's either come with, or you can purchase, solid ferrules (aka: plugs) that will allow you to create a dead end seal at the outlet of the injector).
2. Close the split vent and the septum purge (if applicable).
3. Set the pressure to about 200 kPa (30 psi) for about 30 seconds to pressurize the inlet system. A slight drop to ~193 kPa (~29 psi) is normal within the 3-5 minutes.
4. If you see that the pressure drops rapidly, or drops to 0 within 3-5 minutes, you have a leak.

#### To Fix Suspected Leak(s):

The use of a probe-type leak detector is very helpful in pinpointing helium leaks. But if you do not have a leak detector available, check the following:

1. Septum (Septum is either too loose, has become cored or requires replacement)
2. Column nut/ferrule (Confirm that it's the right size)
3. Terminal fitting silver seal needs to be replaced (never reuse these fittings)
4. Split or purge valve on the flow controller (could be faulty, but unlikely); or
5. Flow controller for cracked weld or bad o-ring (unlikely)

### ARL XRF/XRD Operations

August 16-19, 2007 | Dearborn, MI

This course is designed for new users of the ARL ADVANT'X Series XRF, ARL 9800 XRF/XRD, ARL OPTIM'X XRF, ARL 9900 XRF/XRD and ARL X'TRA XRD instruments that use WinXRF/WinXRD software. Students will learn the skills necessary to operate the instrument and optimize analytical results for their specific applications. Each course is divided into equal portions of lecture and hands-on laboratory time, covering the following topics:

- X-ray theory
- Qualitative/quantitative analysis
- Energy profile
- Sample preparation
- Drift correction
- Inter-elemental correction
- Routine maintenance
- X-ray safety
- Hardware overview
- Evaluation of performance
- High voltage and position calibration
- Liquid analysis
- Calibration/regression analysis
- Fundamental parameters
- Service/parts orientation

Pre-register at [www.thermo.com/education](http://www.thermo.com/education)

### UPCOMING SEMINARS & SHOWS

#### American Society for Mass Spectrometry Meeting

June 3-7, 2007

Indiana Convention Center: BOOTH #54

While you're there, join us in the Thermo Scientific Hospitality Suite!

7:00-10:00 PM (M,T,W)

Indianapolis Marriott Downtown; Ballroom #5

#### 34th Annual FACSS Meeting (Federation of Analytical Chemistry and Spectroscopy Societies)

October 14-18, 2007

Memphis Cook Convention Center; Memphis, TN

For information on all our upcoming seminars & shows Visit:

[www.thermo.com/techtips](http://www.thermo.com/techtips)

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

### Basic Gas Chromatography

August 21-22, 2007 | West Palm Beach, FL

This course is designed for someone with little to no chromatography experience. Students will learn the key fundamentals of gas chromatography, incorporating hands-on experiments using true-to-life samples.

#### Topics include:

- Gas chromatography set-up and requirements
- GC components: Inlets (Split/Splitless, PTV, COC), Detectors (FID, TCD, NPD, ECD, FPD), Injectors (manual injection) and column technology
- Running the instrument (Data collection and viewing)
- Chromatography theory (Plate theory, chromatographic resolution)
- Qualitative and quantitative analysis using GC

Pre-register at [www.thermo.com/education](http://www.thermo.com/education)

**Ask TechTIPS!**

Have a question about your technique, process or method? Then ask! We may feature your question in an upcoming issue.

(All questions submitted become the property of Thermo Fisher Scientific. Questions not published will be answered by one of our highly trained technical specialists.)

Submit your question or comment:  
[www.thermo.com/techtips](http://www.thermo.com/techtips)

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Code: 51394

**2007 Course Schedule**

COURSE TITLE	July	August	September
<b>CHROMATOGRAPHY AND MASS SPECTROMETRY</b> (WEST PALM BEACH, FL; SAN JOSE, CA; BOSTON, MA; KANSAS CITY, MO; LAS VEGAS, NV)			
LCQ Operations	9-12 FL	6-9 FL	10-13 FL
LCQ Biotech Operations	16-19 FL		17-20 FL
LCQ Maintenance			25-27 FL
LTQ XL Operations	9-12 FL	13-16 FL	17-20 FL
LTQ XL Biotech Operations	23-26 FL	6-9 FL	10-13 FL
LTQ XL ETD	30	→ 2 FL	
LTQ Orbitrap Operations	30	→ 2 FL	24-27 FL
LTQ Orbitrap Biotech Operations		20-23 FL	
LTQ FT Ultra Small Molecule Operations (CA)			24-27 CA
LTQ FT Ultra Biotech Operations (CA)			10-13 CA
TSQ Quantum Operations	23-26 FL	27-30 FL	
TSQ Quantum QuickQuan		14-16 FL	
TSQ Quantum LCQUAN	31	→ 2 FL	
MSQ+ Operations (CA)		7-9 CA	
Polaris Q Operations	23-26 FL		10-13 FL
DSQ/DSQ II Operations	9-12 FL	13-16 FL	17-20 FL
ToxLab Operations			5-7 FL
Practical LC/MS for Operations		21-23 FL	
HPLC Method Development for LC/MS Operations	17-18 FL		
BioWorks/SEQUENT® Software Module	2-3 MO		
Xcalibur Software Module	30	→ 1 MO	28-30 FL
Accela HPLC			25-26 FL
MetWorks Software Module		21-22 FL	18-19 MA
EI/CI Interpretation Module	31	→ 2 FL	
Basic Gas Chromatography		21-22 FL	
Gas Chromatography Method Development			25-27 FL

COURSE TITLE	July	August	September
<b>MICROANALYSIS (MADISON, WI)</b>			
NORAN System SIX Operation	24-27 WI		25-28 WI

COURSE TITLE	July	August	September
<b>ELEMENTAL ANALYSIS</b> (WEST PALM BEACH, FL; SCHAUMBURG, IL, MADISON, WI; DEARBORN, MI)			
X Series ICP-MS Operations	17-20 FL	28-31 FL	
iCAP 6000 Series	17-20 FL		25-28 FL
Atomic Absorption		7-10 FL	
IRIS Intrepid ICP Operations	17-20 IL	28-31 IL	
QuantX EDXRF			25-28 WI
XRF Operation		16-19 MI	
OE Operations		13-16 MI	

COURSE TITLE	July	August	September
<b>MOLECULAR SPECTROSCOPY</b> (WEST PALM BEACH, FL; MADISON, WI; SAN FRANCISCO, CA; LAS VEGAS, NV)			
OMNIC™ Software Essentials Operations	17-19 FL		11-13 FL
OMNIC Software Plus Operations		7-10 WI	
FT-IR Spectral Interpretation	24-27 WI		
Fundamentals of FT-IR Analysis		13-17 WI	
Fundamentals of FT-IR Microscopy Operations			17-21 WI
Antaris™ FT-NIR Analyzer Operations			11-13 WI
Centaurus™ Microscope Operations		28-30 FL	
Continuum™ & Continuum XL Microscope Operations	31	→ 3 WI	11-14 WI
Quantitative TQ Analyst Software			18-20 WI
Almega™ Raman Operations (IL; CA)		7-9 IL	
FT Raman Spectroscopy Operations		28-30 WI	
FT-IR Gas Analysis Software	10-12 WI		

Pre-register today at: [www.thermo.com/education](http://www.thermo.com/education) • 1-800-532-4752 • Call us about onsite and customized training!

**Training Institute – North America**

West Palm Beach, FL • Registrar's Office: 1-800-532-4752 • [us.training.analyze@thermo.com](mailto:us.training.analyze@thermo.com)

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For a complete course schedule, visit [www.thermo.com/education](http://www.thermo.com/education)