



Two-day Short Course

“Introduction to LC/MS and LC/MS/MS Mass Spectral Interpretation”

Novatia exists because instrumentation is produced faster than “solutions” or expertise. We are pleased to facilitate this outstanding two day short course. In this course the basics of LC/MS/MS instrumentation and data acquisition are reviewed and a series of tools necessary for interpreting electrospray ionization (ESI) mass spectra and ESI/MS/MS-generated spectra are presented. The course is designed for analysts who are relatively new to mass spectrometry and introduces practiced approaches to interpreting mass spectra. Course examples focus on small molecule applications with ample time provided for hands-on mass spectral interpretation. MS/MS strategies for metabolite, degradant and impurity identification are also presented.

Tues-Wed, April 11-12, 2006
8:30 am - 4:30 pm
Sheraton Bucks County Hotel

Added Bonus - Lunchtime Discussion (Day2):

NMR for structural elucidation often compliments LC/MS. A brief review of the information provided by NMR will be offered. Also presented will be information on new methodologies which are currently becoming available for trace NMR approaches for structure identification.

Novatia is pleased to contract Dr. Cecilia Basic, presenter of the very popular *LC/MS/MS 101* - to teach this course. With over 15 years experience in the fundamentals and applications of mass spectrometry, Dr. Basic has conducted workshops on the principles of mass spectrometry as well as hands-on LC/MS/MS training sessions for pharmaceutical companies and instrument manufacturers. A former professor at Villanova and Lehigh Universities, she has effective teaching materials and a presentation style that walks her students through the fundamentals of this powerful technology.

The details: *The size of the class will be limited.* The cost of this short course is ***\$1,295***. Breakfasts and lunches are included in the course fee. Training materials and a training certificate (including Dr. Basic’s credentials) will also be provided.

To attend: Simply fill out the attached registration form (page 2) and return. A confirmation of your registration will be faxed back to you *within 3 working days*.

***Introduction to LC/MS and LC/MS/MS Mass Spectral Interpretation
2-Day Short Course***

Date: Tues-Wed, April 11-12 , 2006
Location: Sheraton Bucks County Hotel, Langhorne, PA
Time: 8:30 am to 4:30 pm (breakfast at 8:00, start at 8:30)
Cost: \$1,295 per registrant
(5 or more registrants attend for \$995 each)

Registration: If paying by check (make payable to Novatia):

Attn. Kathleen Anderson
11 Deer Park Drive, Suite 202
Monmouth Junction, NJ 08852
(732) 274-9933 x-102

If paying by credit card please do one of the following:

Mail registration form to above address or **fax to (732) 274-9935**

Registrant Information:

Name/Title: _____

Company/Organization: _____

Business Address (incl. mail stop or dept.): _____

City: _____ State: _____ Zip Code: _____

Work Phone: _____ Ext: _____

**** Email address: _____

OR

**** Fax* (Required): _____

**A fax number or email address is required to confirm your reservation and payment.*

Form of Payment:

Check Enclosed (Payable to Novatia)

MasterCard VISA American Express

Credit Card #: _____

Expiration Date: _____

Card Holder Name: _____

Card Holder Signature: _____

2-Day Short Course

Will provide you with the **basic tools necessary in the interpretation of LC/MS and LC/MS/MS mass spectra** generated using the **atmospheric pressure ionization (API) techniques** of electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI) so that you can **confidently begin to interpret mass spectra**.
The course is designed for analysts who are relatively new to MS.

DAY 1

8:30 – 10:15 a.m.

GENERALIZED APPROACH TO MASS SPECTRAL INTERPRETATION

TOOLBOX #1 – SOME GENERAL ORGANIC CHEMISTRY

Chemical Bonding

- Covalent bonds and Lewis symbols
- Octet rule and Single and multiple bonds
- Valences of the Elements
- Lewis Structures and Resonance Structures
- Nitrogen and Double Bond Equivalents Rules

Polyatomic Ions

- Acids and bases

Bond Cleavage in Neutral Molecules

- Heterolytic and Homolytic Cleavage
- Carbocations and carbanions
- Stability and rearrangement of carbocations

Ion Stabilization Processes

- Inductive and resonance stabilization

Isotopes of the Elements

- Isotope classifications
- Calculating isotope patterns and molecular mass

Some Additional Definitions

10:15 – 10:30 a.m. COFFEE BREAK

10:30 a.m. – 12:00 p.m.

TOOLBOX #2 - LC/MS and LC/MS/MS INSTRUMENTS AND METHODS

Overview of LC Mass Spectrometers

Mass Spectrum

Electrospray ionization and Atmospheric Pressure Chemical Ionization

LC/MS vs. LC/MS/MS Mass Spectrometers

- Conventional LC/MS mass spectrometers
- Full-scan MS scans
- Tandem LC/MS/MS mass spectrometers
- Product ion MS/MS scans

Performing product ion scans

- Triple quadrupoles (QqQ), Quadrupole ion traps (QITMS), and Quadrupole time-of-flights (QqTOF)

12:00 – 1:00 p.m. LUNCH

1:00 – 2:30 p.m.

Resolution or resolving power

Isotopic envelopes

- Ion charge state distribution
- Estimating number of C atoms
- Accurate mass measurements

TOOLBOX #3 – SOME GAS PHASE ION CHEMISTRY

Protonated and Deprotonated Molecular Ions
Even-electron (EE^{\pm}) vs. odd-electron (OE^{\pm}) ions
Nitrogen rule for EE^+ molecular ions
Double bond equivalents for EE^{\pm} molecular ions

2:30 – 2:45 p.m. COFFEE BREAK

2:45 – 4:30 p.m.

Location of charge
Gas-phase basicity: Proton Affinity (PA)
Gas-phase acidity: Anion Proton Affinity (APA)
Mobile proton model
Ionization potential (IP)
Ion Energetics
Ionization - ESI and APCI
Ion transport and collision-induced dissociation
CID in MS/MS collision cells

DAY 2

8:30 – 10:15 a.m.

TOOLBOX #4 – ION FRAGMENTATION

Direct cleavage vs. rearrangement
Writing fragmentation mechanisms
General “rules” for low-energy EE^{\pm} fragmentation
Rule (1): stable product ions and logical neutral losses
Rule (2): inductive cleavage
Rule (3): homolytic cleavage
Rule (4): H-rearrangements
Rule (5) and Rule (6)

10:15 – 10:30 a.m. COFFEE BREAK

10:30 a.m. – 12:00 p.m.

INTERPRETING LC/MS and LC/MS/MS Mass Spectra

Generalized Approach
STEP 1: Collect Mass Spectral Information
Full-scan mass spectra
MS/MS product ion scans
STEP 2: Good Quality Mass Spectra
Criteria
STEP3: Compound Information
STEP 4: Identify Molecular Ions
STEP 5: Make Sense of Fragment Ions

BEGIN INTERPRETING MASS SPECTRA

12:00 – 1:00 p.m. LUNCH

1:00 – 2:30 p.m.

COMPLETE INTERPRETING MASS SPECTRA

2:30 – 2:45 p.m. COFFEE BREAK

2:45 – 4:30 p.m.

LC/MS/MS FOR METABOLITE ID BASICS

Common Metabolic Modifications
Screening Biological Samples
Precursor and neutral loss scans
Identifying Drug Modification Sites
Software based metabolite Screening and Identification