



EAS provides low cost, practical problem-solving Short Courses. Various topics will be offered at the 2011 EAS. These courses will be taught by a group of distinguished instructors, who are well recognized in their fields. More details about the preliminary list of Short Courses are provided on the following pages.

Pricing for 2011 Short Courses is \$475 / \$675 before / after Oct. 15<sup>th</sup> for a one-day course and \$675 / \$975 before / after Oct. 15<sup>th</sup> for a two-day course; in addition to the Full Conferee registration fee. Courses are subject to changes.

## Two-Day Courses

Code	Sunday – Monday November 13 - 14	Instructor(s)
E11-01	Practical Gas Chromatography	Dr. Eugene F. Barry, University of Mass- Lowell Dr. Thomas Brettell, Cedar Crest College
E11-02	LC/MS: Theory, Instruments, and Applications	Dr. Guodong Chen, Bristol-Myers Squibb Dr. Michael Balogh, Waters Dr. Ragu Ramanathan, Bristol-Myers Squibb Dr. Birendra Pramanik, Merck
E11-03	Physical Characterization and Analytical Test of Pharmaceutical Solids I & II: Essential Knowledge & Advanced Applications	Dr. Steve R. Byrn, Purdue University Dr. Xiaoming (Sean) Chen, OSI Pharmaceuticals
Code	Monday – Tuesday November 14 - 15	Instructor(s)
E11-12	How to Develop Validated HPLC Methods: Rational Design with Practical Statistics and Troubleshooting	Dr. Brian A. Bidlingmeyer, Agilent Technologies Dr. Stanley N. Deming, Statistical Designs
E11-13	Putting Organic Chemistry into Perspective - A Review of Sophomore Organic Chemistry	Dr. John R. Sowa, Seton Hall University
E11-14	Infrared Spectral Interpretation I + II ( <i>combined course</i> )	Dr. Brian C. Smith, Spectos Associates
Code	Tuesday – Wednesday November 15 - 16	Instructor(s)
E11-21	The Analysis and Characterization of Protein Therapeutic Drugs	Mr. C. David Carr, Bioanalytical Technologies
Code	Wednesday – Thursday November 16 - 17	Instructor(s)
E11-29	Troubleshooting Chromatographic Systems	Dr. Merlin K.L. Bicking, ACCT, Inc. Dr. Douglas E. Raynie, South Dakota State University
E11-30	Hands-on FTIR, NIR and Data Analysis – What is the Right Tool to Solve Your Problem	Dr. Katherine A. Bakeev, CAMO Software Dr. Brian C. Smith, Spectros Associates
E11-31	Essentials of Modern HPLC I & II ( <i>combined course</i> )	Dr. Michael W. Dong, Genentech

## One-Day Courses

Code	Sunday, November 13	Instructor(s)
E11-04	Physical Characterization and Analytical Test of Pharmaceutical Solids I: Essential Knowledge	Dr. Steve R. Byrn, Purdue University Dr. Xiaoming (Sean) Chen, OSI Pharmaceuticals
E11-05	<del>Effective Laboratory Audits and Inspections</del>	Cancelled
E11-06	Intermediate Chemometrics Without Equations	Dr. Donald Dahlberg, Lebanon Valley College Dr. Barry M. Wise, Eigenvector Research
E11-07	<del>Modern HPLC Method Development in Pharmaceutical Analysis</del>	Cancelled
E11-08	Enhanced Productivity by Design in the Analytical Laboratory: Design of Experiments for Analytical Chemists	Dr. Zenaida Otero Gephardt, Rowan University
E11-09	Impurities and Degradants Identification: Strategies for Structure Elucidation via Chromatography, MS and NMR	Dr. Thomas R. Sharp, Pfizer Dr. Brian L. Marquez, Pfizer Mr. Todd C. Zelesky, Pfizer
E11-10	Impurities in Pharmaceuticals - A Survey Course <b>(NEW)</b>	Dr. Bernard A. Olsen, Olsen Pharmaceutical Consulting
E11-11	Polymers: An Introduction and Characterization Techniques <b>(NEW)</b>	Dr. Diep Nguyen, Illinois Institute of Technology

<b>Code</b>	<b>Monday, November 14</b>	<b>Instructor(s)</b>
E11-15	Infrared Spectral Interpretation I	Dr. Brian C. Smith, Spectros Associates
E11-16	Critical cGMP and ICH Guidances for Analytical Laboratories	Ms. Kim Huynh-Ba, US Pharmacopeia Dr. Linda Ng, US Food and Drug Administration
E11-17	Physical Characterization and Analytical Test of Pharmaceutical Solids II: Advanced Applications	Dr. Steve R. Byrn, Purdue University Dr. Xiaoming (Sean) Chen, OSI Pharmaceuticals
E11-18	Analytical Laboratory Techniques for Analytical Laboratory Staff	Dr. Merlin K.L. Bicking, ACCTA, Inc.
E11-19	Laboratory Data Analysis Using Excel <sup>®</sup> : New Uses for a Familiar Tool	Dr. Zenaida Otero Gephardt, Rowan University
E11-20	Concepts in Sustainability and Green Chemistry <b>(NEW)</b>	Dr. Douglas E. Raynie, South Dakota State University
<b>Code</b>	<b>Tuesday, November 15</b>	<b>Instructor(s)</b>
E11-22	The Role of Chromatography in the Analysis and Characterization of Protein Therapeutic Drugs	Mr. C. David Carr, Bioanalytical Technologies
E11-23	Infrared Spectral Interpretation II	Dr. Brian C. Smith, Spectros Associates
E11-24	Sample Preparation: The Chemistry Behind the Techniques	Dr. Merlin K.L. Bicking, ACCTA, Inc. Dr. Douglas E. Raynie, South Dakota State University
E11-25	Introduction to Near-Infrared Spectroscopy: Applications in the Pharmaceutical and Biotech Industries	Dr. Emil Ciurczak, Doramaxx Consulting
E11-26	<del>How to Create a More Effective Lab Safety Program</del>	Cancelled
E11-27	Data Analysis for Improved Productivity in the Analytical Laboratory	Dr. Zenaida Otero Gephardt, Rowan University
E11-28	Interpretation of Mass Spectra with Practical Solutions to Problems	Dr. Birendra Pramanik, Merck Dr. Mike Lee, Milestone Development
<b>Code</b>	<b>Wednesday, November 16</b>	<b>Instructor(s)</b>
E11-32	Essentials of Modern HPLC I: Fundamentals and Applications	Dr. Michael W. Dong, Genentech
E11-33	Anatomy of Modern Reversed-Phase Columns: Understanding Their Role in HPLC	Dr. Brian A. Bidlingmeyer, Agilent Technologies Dr. Richard A. Henry, Penn State University
E11-34	Practical Headspace Gas Chromatography	Dr. Mary Ellen P. McNally, DuPont Dr. Thomas A. Brettell, Cedar Crest College
E11-35	Analytical Metrology <b>(NEW)</b>	Dr. Jerry D. Messman, Stranaska Scientific
E11-36	<del>High-Throughput Drug Analysis by LC/MS <b>(NEW)</b></del>	Cancelled
E11-37	<del>Practical Enantiomeric Separations <b>(NEW)</b></del>	Cancelled
E11-38	Residual Solvents Testing: Strategies to Meet the USP <467> Requirements <b>(NEW)</b>	Mr. Gregory Martin, Complectors Consulting
E11-39	Fundamentals of Gas Chromatography for New Analysts and Non-Chemists <b>(NEW)</b>	Dr. Harold McNair, Virginia Tech Dr. Nicholas Snow, Seton Hall University
<b>Code</b>	<b>Thursday, November 17</b>	<b>Instructor(s)</b>
E11-40	Essentials of Modern HPLC II: Practice, Operation, Troubleshooting and Method Development	Dr. Michael W. Dong, Genentech
E11-41	Quantitative Analysis for Managers, Auditors and Data Reviewers <b>(NEW)</b>	Dr. Nicholas Snow, Seton Hall University Dr. Gregory Slack, Clarkson University
E11-42	Practical Solutions to Characterization of Protein Therapeutics Using Mass Spectrometry	Dr. Guodong Chen, Bristol-Myers Squibb Dr. Li Tao, Bristol-Myers Squibb
E11-43	Practical Introduction to Raman Spectroscopy	Dr. Frederick H. Long, Spectroscopic Solutions
E11-44	Dissolution: A Rational Approach to Developing and Validating Methods for a Variety of Purposes	Mr. Gregory Martin, Complectors Consulting
E11-45	<del>Introduction to Metabolomics <b>(NEW)</b></del>	Cancelled
E11-46	Detection and Characterization of Drug Metabolites in Drug Discovery and Development <b>(NEW)</b>	Dr. Donglu Zhang, Bristol-Myers Squibb Dr. Mingshe Zhu, Bristol-Myers Squibb
E11-47	The Chemistry of Drug Degradation	Dr. Karen Alsante, Pfizer Dr. Dinos Santafricanos, Pfizer

## EAS Short Courses

EAS Short Courses emphasize practical and economical problem-solving topics which will include material that you can take home and immediately apply to your daily work. Various topics will be offered at the 2011 EAS. These courses will be taught by a group of distinguished instructors, who are well recognized in their fields.

Please visit [www.EAS.org](http://www.EAS.org) to register.

### Practical Gas Chromatography

**Two-Day Course E11-01. Sunday and Monday, November 13 and 14, 2011, 8:30am-5:30pm**

Dr. Eugene F. Barry, University of Massachusetts Lowell, Lowell, MA

Dr. Mary A. Kaiser, DuPont Company, Wilmington, DE

#### COURSE DESCRIPTION

This course presents the fundamentals of gas chromatography with an emphasis on practical applications for users and method developers. Topics to be covered include theoretical considerations, use of computer searches for literature references and methods of analysis, modern instrumentation, including inlet, column, and detector technology, and the applications of these to effective qualitative and quantitative analysis. The theoretical portion of the course will focus on using the fundamental understanding of the chromatographic process (limited number of equations and comparisons to extractions and distillations) to assist in obtaining a desired separation quality and run time. Modern instrumentation including split, splitless, on-column, and programmed-temperature inlets and electronic pressure control will be discussed. The proper selection of capillary columns to solve practical problems will be described, although the utility of modern packed columns will be briefly discussed. An emphasis will also be placed on detectors, including TCD, FID, ECD and GC/MS. Finally all this will be applied to practical problems in qualitative and quantitative analysis.

#### WHO SHOULD ATTEND

This course represents a balanced blend of pertinent information and underlying theory for successful practice of gas chromatography. Individuals working in the area of gas chromatography, beginners and those desiring to update their knowledge of the technique will find this course to be meaningful and useful. The Instructors of this Short Course will welcome Questions and Problems pertinent to the subject material covered in the course prior to the Meeting. These Questions & Problems will be answered in a Question & Answer Session at the end of the Course. Email your inquiries to either of the two Instructors: Dr. Eugene F. Barry: [Eugene\\_Barry@uml.edu](mailto:Eugene_Barry@uml.edu) or Dr. Mary A. Kaiser: [Mary.A.Kaiser@usa.dupont.com](mailto:Mary.A.Kaiser@usa.dupont.com).

#### TOPICS

- ▶ Theory and Basics
  - Evolution of chromatography
  - IUPAC nomenclature
  - Similarities to extractions & distillations
  - Theory of gas chromatography-Plate and Rate Theories
  - Effect of changing conditions on peak separations
- ▶ Inlets/mobile Phases
  - Injection modes & mobile phases
  - Instrumental requirements for packed and capillary columns
  - Capillary column inlets (split, splitless, on-column, direct injection, electronic pressure control)
  - Programmed-temperature vaporizer, large volume injections.
  - Packed column inlets /column selection
  - Classification and selection of stationary liquid phases and adsorbents
  - Capacity and analysis time
- ▶ Capillary Column
  - Capillary column selection
  - Chromatographic parameters affecting column performance
  - Effect of capillary column ID, film thickness, length & choice of carrier gas on resolution
  - Capillary column rinsing, rejuvenation, care and maintenance
- ▶ Detectors
  - Fundamentals of detector responses
  - Types of detectors
  - Detectors used for various analysis
- ▶ Computer Assistance in Gas Chromatography
  - Internet guidance
  - Software for prediction and optimization of separations
- ▶ Qualitative and Quantitative Analysis
  - Qualitative analysis
  - Quantitative analysis methods

\*NOTE: This course covers gas chromatography, not the technique of gas chromatography-mass-spectrometry (GC-MS). *Modern Practice of Gas Chromatography; 4th Edition*, Robert L. Grob and Eugene F. Barry, Eds.; John Wiley & Sons: New York, 2004. ISBN 0-471-22983-0

### **ABOUT THE INSTRUCTORS**

**Dr. Eugene F. Barry** is Professor of Chemistry and Chairman of the Chemistry Department at the University of Massachusetts Lowell. He received his B.S. in Chemistry from Villanova University (1967) and a Ph.D. in Analytical Chemistry from the University of Rhode Island (1970). In collaboration with the late Robert L. Grob, he is co-editor of *Modern Practice of Gas Chromatography*, Fourth Edition and co-author of the book, *Columns for Gas Chromatography: Performance and Selection*, both published by John Wiley. He has taught at the Pittsburgh Conference and the Eastern Analytical Symposium. During his tenure at the University of Massachusetts Lowell, Dr. Barry has taught a wide variety of courses in Analytical Chemistry, including graduate level courses in chromatography and separation methods, his primary area of research. His current research interests include GC-MS, computer-assisted optimization of separations by capillary GC, high-speed gas chromatography, enhanced oil recovery in addition to geological and oceanic sequestration of carbon dioxide and the determination of organics in challenging matrices, such as cement and concrete. He is author of over 100 research publications and several patents.

**Dr. Mary A. Kaiser** is a Senior Research Fellow in DuPont's Corporate Center for Analytical Sciences in Wilmington, Delaware. She received the Ph.D. under the direction of Dr. Robert L. Grob from Villanova University. She has over years of analytical science experience in industry. She co-authored a book on environmental analysis using GC and LC and has published over 55 papers and given over 95 technical presentations. She taught at the University of Delaware, the Society of Environmental Toxicology and Chemistry, the Chromatography Forum of the Delaware Valley, the Pittsburgh Conference and the Eastern Analytical Symposium. She served as President of the Chromatography Forum of the Delaware Valley, FACSS governing board chair, chair of the Division of Analytical Chemistry, American Chemical Society and President of EAS. She was awarded the Villanova University Founders Award, the Chromatography Forum of the Delaware Valley Award, the ACS Division of Analytical Chemistry service award, and the Delaware Section ACS award.

This course is dedicated to the late Dr. Robert Grob in honor to his years of service to academics, industry, the GC community and Eastern Analytical Symposium.

## **LC/MS: Theory, Instruments and Applications**

***Two-Day Course E11-02, Sunday and Monday, November 13 and 14, 2011, 8:30am-5:30pm***

Dr. Guodong Chen, Bristol-Myers Squibb, Princeton, NJ  
 Mr. Michael Balogh, Waters Corporation, Milford, MA  
 Dr. Ragu Ramanathan, Bristol-Myers Squibb, Princeton, NJ  
 Dr. Birendra N. Pramanik, Merck and Co., Kenilworth, NJ

### **COURSE DESCRIPTION**

This course is designed to be an introduction to the theory and practical implementation of LC/MS and LC/MS/MS technology in the laboratory. It emphasizes problem-solving skills with examples encountered in industrial and academic research including characterization of trace level drug substance impurities and degradation products, identification of drug metabolites, and the analysis of natural products and bio-molecules. The interpretation of mass spectra will be illustrated with practical examples. In addition, structure determination of proteins and peptides will be presented. This course will focus on atmospheric pressure ionization interfaces including electrospray and atmospheric pressure chemical ionization, and will survey the various mass analyzer options. This course will address issues regarding the coupling of capillary HPLC, microbore HPLC, and standard 4.6 mm chromatography. A thorough coverage of approaches toward method development for both qualitative and quantitative analysis of pharmaceutical products and biopolymers will provide a good starting point for understanding the practical issues facing implementation of LC/MS in the laboratory. Furthermore, an overview of the current state-of-the-art of automating the LC/MS laboratory including the interfacing of automated sample preparation devices will be provided. Finally, this course will cover technological advancement in biological mass spectrometry combined with separation techniques for analyzing proteins and peptides.

### **WHO SHOULD ATTEND**

This course is designed for practicing LC/MS chemists (new users, chromatographers, analytical chemists, protein chemists, and laboratory managers).

### **TOPICS**

- ▶ Introductions to Liquid Chromatography (LC) / Mass Spectrometry (MS)
  - History
  - Instrument overview: sector, ion trap and TOF
- ▶ Introductory Theory
  - Ionization
  - Electron ionization (EI)
  - Atmospheric pressure ionization API (ESI, APCI)
- ▶ Mass Analyzers
  - Quadrupoles
  - Magnetic sectors
  - Ion trap
  - Ion cyclotron resonance (ICR)
  - Time-of-flight
  - Orbitrap
- ▶ LC/MS Method Development

- ▶ • Issues
    - Electrospray ionization (ESI)
    - Atmospheric pressure chemical ionization (APCI)
  - ▶ Automation and High Throughput Sample Analysis
    - Sample preparation
    - Development of high-throughput chromatography
  - ▶ Tandem Mass Spectrometry (MS/MS) and LC/MS/MS
  - ▶ Sample Preparation for LC/MS
- ▶ Application in Drug Metabolism
  - ▶ Applications—Small Molecules, Pharmaceuticals, Natural Products (Structure Elucidation, Identification and Quantitation)
  - ▶ Applications—Proteins and Peptides
    - Protein characterization and structural problems
    - Non-covalent interactions and drug discovery process
    - Proteomic

### ABOUT THE INSTRUCTORS

**Dr. Guodong Chen** (Course Director) has extensive pharmaceutical research experience in major pharmaceutical companies, including Eli Lilly and Co., Schering-Plough (now Merck) and Bristol-Myers Squibb. He is currently heading a mass spectrometry group at Bristol-Myers Squibb's Princeton site, providing mass spectrometric/analytical support to drug discovery and development programs in small molecule pharmaceuticals and biologics. He is the author and/or co-author of over 50 research publications in peer-reviewed journals and book chapters, covering the broad area of mass spectrometry and analytical sciences. He has over 65 presentations at conferences and academic institutes. He also organized/chaired scientific sessions at various forums, including major sessions on small molecule pharmaceuticals and biologics at EAS, Pittcon, ASMS conference and ACS conference. Dr. Chen was the Chairperson of the North Jersey Section of ACS Mass Spectrometry Discussion Group (2004) and in 2006, he received Early Career Award in Mass Spectrometry. He was an invited Analytical Chemistry Program Chair for ACS MARM Conference (2005) and elected President of Chinese American Chemical Society-Tri State (2007). He serves as founding coordinator for ASMS Protein Therapeutics Interest Group (2009-2011). Dr. Chen received his Ph.D. in Analytical Chemistry from Purdue University under the direction of Professor R. Graham Cooks.

**Mr. Michael Balogh** is a Principal Scientist in MS Technology Development at Waters Corporation. He has held the position of adjunct professor and visiting scientist at Roger Williams University and has been a reviewer for grant proposals for the National Science Foundation (NSF). His current interests involve improvements in atmospheric source design and multi-mode ionization for mass spectrometry, an area where he has developed patented technology. From 1995 to 2004, Michael was chair and co-organizer of liquid chromatography/mass spectrometry (LC/MS) interest group for the American Society for Mass Spectrometry (ASMS). His work over the past 20 years has appeared in the Journal of Nuclear Medicine, Journal of Chromatography, Analytical Chemistry, LCGC, Rapid Communications in Mass Spectrometry among others. He has taught courses in LC/MS fundamentals and practice and provides a column, MS – The Practical Art, which appears regularly in LCGC both in North America, Europe and Asia and is on their scientific advisory board. He is also co-founder and currently president of the Society for Small Molecule Science which organizes the Conference on Small Molecule Science.

**Dr. Ragu Ramanathan** is a Senior Principal Scientist in the Department of Biotransformation at Bristol-Myers Squibb Co., Princeton, NJ. He previously worked at Schering-Plough Research Institute (now Merck) and Warner-Lambert (now Pfizer). Dr. Ramanathan earned his Ph.D. and BS from the University of Florida (Gainesville, FL) and the University of Southern Mississippi (Hattiesburg, MS), respectively. Dr. Ramanathan's primary focus of research involves application of LC-MS for pharmaceutical drug discovery and development...

## Physical Characterization and Analytical Test of Pharmaceutical Solids I and II: Essential Knowledge and Advanced Applications

**Two-Day Course E11-03, Sunday and Monday, November 13 and 14, 2011, 8:30am-5:30pm**

Dr. Steve R. Byrn, Purdue University, West Lafayette, IN  
Dr. Xiaoming (Sean) Chen, OSI Pharmaceuticals, Inc, Cedar Knolls, NJ

### COURSE DESCRIPTION

This course is a combination of two one-day courses: Physical Characterization and Methods of Analysis of Pharmaceutical Solids I and II. A discount will be offered over separately registering for the two one-day courses.

### WHO SHOULD ATTEND

This two-day course will benefit formulation scientists, process engineers, analysts, QA and QC managers, regulators, and researchers, who perform process development and manufacture of drug substances, develop formulations of drug products, conduct analytical testing and method development, set up stability programs, and evaluate stability data of drug substances and products.

### TOPICS

#### **DAY ONE:**

- See Topics listed under Physical Characterization and Analytical Test of Pharmaceutical Solids I: Essential Knowledge

#### **DAY TWO:**

- See Topics listed under Physical Characterization and Analytical Test of Pharmaceutical Solids II: Advanced Applications

### ABOUT THE INSTRUCTORS

See instructor information under Physical Characterization and Analytical Test of Pharmaceutical Solids I and II course descriptions above.

## **Physical Characterization and Analytical Test of Pharmaceutical Solids I: Essential Knowledge**

**One-Day Course E11-04, Sunday, November 13, 2011, 8:30am-5:30pm**

Dr. Steve R. Byrn, Purdue University, West Lafayette, IN  
Dr. Xiaoming (Sean) Chen, OSI Pharmaceuticals, Inc, Cedar Knolls, NJ

### COURSE DESCRIPTION

Physical characterization and methods of analysis of pharmaceutical solids are essential for drug research and development. Solid characteristics such as polymorphism, formation of hydrate and solvate, and crystallinity have profound impact on the quality attributes of drug substances and drug products such as solubility, dissolution, bioavailability, processability, and stability. Characterization of those solid state properties is critical for selection and manufacture of desirable solid forms for development. This short course presents some essential knowledge for pharmaceutical solids. It also introduces methods of analysis of the solid state such as X-Ray powder diffraction, differential scanning calorimetry, thermogravimetric analysis, microscopy, infrared spectroscopy, Raman spectroscopy, and solid state NMR. Applications of those techniques in the final form selection of drug substances and mixture analysis of drug products are discussed.

### WHO SHOULD ATTEND

This one-day course will benefit formulation scientists, process engineers, analysts, QA and QC managers, regulators, and researchers, who perform process development and manufacture of drug substances, develop formulations of drug products, conduct analytical testing and method development, set up stability programs, and evaluate stability data of drug substances and products.

### TOPICS

- ▶ **Pharmaceutical Solids—Introduction**
  - Polymorphs
  - Solvates and hydrates
  - Salt formation and co-crystal
  - Amorphous forms
- ▶ **Methods of Analysis**
  - Crystal packing, unit cell, X-ray powder diffraction
  - Differential scanning calorimetry and thermogravimetric analysis
  - Microscopy
  - Infrared spectroscopy and Raman spectroscopy
  - Solid-state NMR

### ABOUT THE INSTRUCTORS

**Dr. Stephen R. Byrn** is Charles B. Jordan Professor of Medicinal Chemistry in the School of Pharmacy, Purdue University, West Lafayette, Indiana. He is also Head of the Department of Industrial and Physical Pharmacy. He received his B.A. degree in Chemistry from DePauw University and his Ph.D. degree in Chemistry from the University of Illinois, Urbana. He did postdoctoral research at UCLA. His research focuses on solid state chemistry, polymorphism, stability, manufacturing science, quality by design, and medicinal chemistry. Dr. Byrn opened up the field of solid state chemistry of drugs with his research and books of that title (first edition, 1982, second edition, 2000). Dr. Byrn has founded and directed several programs at Purdue University including CAMP, the Center for AIDS Research, the Molecules to Market program, and Purdue's graduate programs in regulatory and quality compliance. He is also one of the founders and a member of the executive committee of NIPTE (National Institute for Pharmaceutical Technology and Education). He continues to be involved in educating scientists in solid state chemistry, methods of analysis, and regulatory science. Dr. Byrn has served as chair of the Pharmaceutical Sciences Advisory Committee to the FDA and Chair of the Drug Substances Technical Committee, Product Quality Research Initiative. Dr. Byrn has extensive experience as a consultant in the pharmaceutical industry and currently serves as Purdue's representative to the USP. Dr. Byrn is co-founder of SSCI, Inc. (Solid State Chemical Information) a cGMP research and information Company specializing in polymorphism, crystallization, analysis, problem solving and regulatory issues. SSCI, Inc. is now owned by Aptuit and Dr. Byrn serves as Head of the Aptuit Scientific Advisory Board. Dr. Byrn is also a technical founder of Andara now owned by Cyberkinetics, Inc. Andara specializes in devices and drugs for the treatment of spinal cord injury and CNS diseases.

**Dr. Xiaoming (Sean) Chen** received his Ph.D. in Industrial and Physical Pharmacy from Purdue University in 2000. He has worked as a project leader in discovery support and preformulation at Schering-Plough Research Institute for five years. He has contributed the nomination of five NCE for development and received one President Award, one Impact Award and Three Excellence Awards from Schering-Plough Research Institute. He has also worked in Exploratory Formulation group of Schering-Plough for three years, leading formulation development of two important line extension projects. Currently, Dr. Chen is a Senior Development Investigator in Pharmaceutical Development of OSI Pharmaceuticals. Dr. Chen is an expert in physical characterization of solids, crystal form and salt selection, and controlled

release formulation. He has published over a dozen of papers in peer-reviewed journals. Dr. Chen is a member of AAPS and has served in PDD award committee for two years.

## Effective Laboratory Audits and Inspections

**One-Day Course E11-05, Sunday, November 13, 2011, 8:30am-5:30pm**

Mr. Kenneth Christie, VTS Consultants, Inc., Amherst, MA

### COURSE DESCRIPTION

A vital part of a quality system is the requirement for auditing of suppliers to assure their quality practices meet the expectations of one's company. In an attempt to reduce costs, companies today are increasingly outsourcing both needed services and expanding their dependency on suppliers. Laboratories, based on the data they provide that impacts the use of raw materials and components or the release of final products is an increasing area of focus during regulatory inspections. This course will help provide a template in terms of how to audit such suppliers, manufacturers and laboratories that many companies depend on. It will focus on current regulatory expectations and responsibilities for these audits, along with reviewing the main points to cover during the audit. The course will examine expectations as defined in 21 CFR 58, and ISO 17025. Auditing do's and don'ts will be covered and participants will be given a chance to raise questions regarding their current practices and procedures.

### WHO SHOULD ATTEND

This one-day course will benefit laboratory analysts, QA and QC managers, regulators, and manufacturers, who depend on various services or products that are performed or obtained by outside services or suppliers. Companies must remember that they are responsible for the quality of these services or components as they are the ones who are ultimately liable for the end product.

### TOPICS

- ▶ Regulatory Requirements and Guidelines.
  - Review of expectations as defined in 21 CFR 58.
  - Review of common industry practices as recommended by ISO 17025.
  - Discuss the main objectives for conducting audits.
- ▶ Preparing for Audits of Suppliers/Labs.
  - Learn how to prepare for conducting an audit and assembling the audit team.
  - Define the areas to be audited per a check list.
  - Review the main areas of focus and typical areas of deficiencies.
- ▶ Review Practices Required for an Effective Audit Program.
  - Review do's and don'ts during the audit.
  - Prepare final report and classifications of findings.
  - Discuss follow-up activities for marginally acceptable suppliers.
  - Discuss regulatory ramifications for non-acceptable suppliers.
- ▶ Interactive Exercises and Discussion - Participants will openly discuss questions associated with their current auditing practices or have questions answered regarding results.

### ABOUT THE INSTRUCTOR

**Mr. Kenneth Christie** has over 20 years of sterile manufacturing experience in the areas of Quality Assurance and Validation Management in the pharmaceutical and biotechnology industries. Mr. Christie is currently the Chief Operating Officer for VTS Consultants, Inc located in Amherst, MA. He is responsible for both business development planning and Validation and Regulatory Consulting services on a global basis. Specifically, his responsibilities include quality system auditing, GMP training, and serving as a subject matter expert for aseptic and solid dosage processing equipment, utilities, and systems.

Prior to joining VTS, Mr. Christie was the Validation Manager at Parke-Davis' Sterile Products Facility in Rochester, MI. While there, he was involved in the review and approval of all facility, equipment, and system commissioning/qualification activities. Additional responsibilities included routine interaction with the FDA and European inspectors, corporate management and third party contract-manufacturing representatives to defend validation practices and to assure regulatory compliance for the manufacture of aseptically produced products.

Mr. Christie is a speaker and trainer for several professional organizations in the US, Canada, Europe, and Asia and is a published author of several articles dealing with the challenges of aseptic processing. Additionally, Mr. Christie serves as a member of the ISPE Professional Certification (PCC) Commission Examination Development Committee (EDC), which is industry's first attempt to "certify" industry professionals based on proven regulatory knowledge. He possesses a BS degree in Biology from Shippensburg State University (PA) and an Executive MBA degree from Michigan State.

## Intermediate Chemometrics Without Equations

**One-Day Course E11-06, Sunday, November 13, 2011, 8:30am-5:30pm**

Dr. Donald Dahlberg, Lebanon Valley College (Emeritus), Annville, PA  
Dr. Barry M. Wise, Eigenvector Research, Wenatchee, WA

### COURSE DESCRIPTION

This course concentrates on two areas of chemometrics: (1) data pretreatment and (2) mixture analysis. No process is more important to the success of a chemometric model than the use of the appropriate pretreatment of the data. Participants learn the common sources of nonlinearity and extraneous variation in spectral data and how to remove these artifacts with the appropriate pretreatment. Emphasis is put on how each pretreatment works, which leads to an understanding of the advantages, disadvantages and proper application of each technique. Multivariate Curve Resolution (MCR) and Self-modeling Mixture Analysis (SMA) are powerful chemometric techniques that allow the user to determine the composition profile and the pure component spectra of a mixture. These techniques have been applied to resolving overlapping peaks in hyphenated chromatography and determining the time or spatial distribution of substances in reactions and heterogeneous mixtures.

### WHO SHOULD ATTEND

This course on Chemometrics Without Equations (or Hardly Any) is designed for those who wish to explore the problem-solving power of chemometric tools, but are discouraged by the high level of mathematics found in many software manuals and texts. Course emphasis is on proper application and interpretation of chemometric methods as applied to real-life problems. The objective is to teach in the simplest way possible so that participants will be better chemometrics practitioners and managers.

### TOPICS

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| <ul style="list-style-type: none"> <li>▶ Introduction           <ul style="list-style-type: none"> <li>• What is chemometrics</li> <li>• Resources</li> </ul> </li> <li>▶ Pattern Recognition Motivation           <ul style="list-style-type: none"> <li>• What is pattern recognition</li> <li>• Relevant measurements</li> <li>• Some statistical definitions</li> </ul> </li> <li>▶ Principal-component Analysis           <ul style="list-style-type: none"> <li>• What is PCA</li> <li>• Scores and loadings</li> <li>• Interpretation</li> <li>• Supervised and unsupervised pattern recognition</li> <li>• Examples</li> </ul> </li> </ul> | <ul style="list-style-type: none"> <li>▶ Regression           <ul style="list-style-type: none"> <li>• What is regression</li> <li>• Classical least squares (CLS)</li> <li>• Inverse least squares (ILS)</li> <li>• Principal components regression (PCR)</li> <li>• Partial least squares regression (PLS)</li> <li>• Examples</li> </ul> </li> <li>▶ On-line Application           <ul style="list-style-type: none"> <li>• Clients and servers</li> <li>• Available technologies (COM, ActiveX, etc.)</li> <li>• Using MATLAB and PLS_Toolbox on line</li> </ul> </li> <li>▶ Summary</li> </ul> |
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### ABOUT THE INSTRUCTORS

**Dr. Donald Dahlberg** (Course Director) is Professor Emeritus of Chemistry at Lebanon Valley College. Dr. Dahlberg earned a B.S. in Chemistry from the University of Washington and a Ph.D. in Physical Chemistry from Cornell University. After decades of doing research in the area of Physical Organic Chemistry, he got involved in Chemometrics while on sabbatical in 1988 at the Center for Process Analytical Chemistry at the University of Washington. There he learned chemometrics in the Bruce Kowalski group (co-founder of chemometrics). Upon returning to LVC, he taught chemometrics to undergraduate students for over a decade. Although retired from the classroom, he continues to do consulting and supervises undergraduate research in industrial chemometrics. Dr. Dahlberg wrote and teaches this course so that those not fluent in matrix algebra can take advantage of the powerful tool of chemometrics.

**Dr. Barry M. Wise**, PLS\_Toolbox creator and co-founder of Eigenvector Research, holds a doctorate in Chemical Engineering and has experience in a wide variety of applications spanning chemical process monitoring, modeling and analytical instrument development. He has extensive teaching experience, having presented over 50 chemometrics courses.

## Modern HPLC Method Development in Pharmaceutical Analysis

**One-Day Course E11-07, Sunday, November 13, 2011, 8:30am-5:30pm**

Dr. Michael W. Dong, Genentech, Small Molecule Analytical Chemistry, S. San Francisco, CA  
Dr. Henrik T. Rasmussen, Vertex Pharmaceuticals, Cambridge, MA

### COURSE DESCRIPTION

This is a one-day HPLC method development course at an intermediate/advanced level. The course reviews relevant concepts, best practices and tricks-of-the-trade to help the attendees to become more successful in developing difficult ICH-compliant stability-indicating

HPLC methods for pharmaceuticals (small-molecule drug substances and products). The focus is on methods for new chemical entities, complex molecules with one or more chiral centers, and drug products with multiple APIs. Though case studies are taken from pharmaceutical analysis, concepts presented in this course would be useful to attendees from other industries.

### WHO SHOULD ATTEND

This course is intended for analysts, managers, regulators and researchers using HPLC in the pharmaceutical laboratory (or other industries). At least two (2) years of practical hands-on experience is suggested as a prerequisite.

### TOPICS

- ▶ Course Introduction/Overview
- ▶ Key Concepts and Modern Trends in HPLC Method Development
  - Common-sense but often-neglected corollaries in HPLC separations
  - Practical concepts ( $k'$ ,  $\alpha$ ,  $n$ ,  $R_s$ ,  $V_M$ , peak volume,  $H$ ,  $dp$ , method orthogonality), and mobile phase parameters (organic modifiers, pH)
  - Column fundamentals and selection
  - UV detector fundamentals and wavelength selection
  - Important instrumental considerations: system dispersion and dwell volume
  - Modern trends in method development
- ▶ ICH Guidelines
  - ICH guidelines Q2A, Q2B, Q3A, Q3B and interpretation
- ▶ The Traditional Method Development Approach and Case Studies
  - Defining method types/goals and gathering pertinent sample / analyte information
  - Scouting gradient and getting the first chromatogram
  - Method fine-tuning and optimization (Solvent strength/type, pH, buffer/additive, F, T,  $t_G$ , column screening)
  - Demonstrating method specificity and stability-indicating capability (how to conduct rapid forced degradation studies)
  - Use of simulation software to facilitate selectivity tuning and column optimization
- Final method adjustments for ICH compliance methods (peak shape, LOQ, analysis time)
- Case studies for NCEs, complex formulations and drug products with multiple APIs
- ▶ Phase Appropriate Method Development and Validation
  - Forced decomposition studies
  - Development of orthogonal methods
  - Progressive validation strategies
- ▶ The 3-Prong Approach and Tools for Efficient Method Development
  - Road map for efficient method development - the 3-prong approach (Generic IPC gradients, Fast LC isocratic, multi-segment gradients)
  - Automated column and mobile phase screening systems
  - Case study on method support for molecules with multiple chiral centers using achiral and chiral methods to assess and control starting materials, intermediates and final APIs
- ▶ Method Robustness Testing
  - Critical control parameters for HPLC
  - Use of Experimental designs for establishing Robustness
- ▶ New Developments in HPLC
  - HILIC, monolith, sub-3  $\mu\text{m}$  and sub-2  $\mu\text{m}$  packing, fused core particles, ultra high-pressure LC, high-temperature LC, parallel analysis, Lab-on-a-chip

### RECOMMENDED TEXT

1. L. R. Snyder, J. J. Kirkland & J. L. Glajch, *Practical HPLC Method Development*, 2nd Ed., Wiley-Interscience, NY, 1997.
2. M. W. Dong, *Modern HPLC for Practicing Scientists*, Wiley, New Jersey, June 2006.
3. S. Ahuja and H. Rasmussen (ed.), *HPLC Method Development for Pharmaceuticals*, Academic Press, 2007.

### ABOUT THE INSTRUCTORS

**Dr. Michael W. Dong** (Lead instructor) is a Senior Scientist at Genentech, Small Molecule Drug Discovery, South San Francisco, CA. His research interests are in Fast LC, ultra-high-pressure LC, rapid HPLC method development and chiral separations. He was formerly Research Director at Synomics Pharmaceutical Services, Research Fellow/Group Leader at Purdue Pharma, Senior Staff Scientist at Applied Biosystems / Perkin-Elmer, and section-head in Hoechst Celanese. He holds a B.Sc. in Chemistry from Brooklyn College and a Ph.D. in Analytical Chemistry from City University of New York Graduate Center. He has conducted numerous HPLC training courses at national meetings (ACS, PittCon, EAS, AAPS) on advanced HPLC, Fast LC / HTS, stability testing and HPLC method development. He pioneered Fast LC and has over 80 publications in chromatography, pharm analysis and analytical chemistry. He authored a best-seller in chromatography – “Modern HPLC for Practicing Scientists”, Wiley, 2006 and co-edited Handbook of Pharmaceutical Analysis by HPLC, Elsevier/Academic Press, 2005.

**Dr. Henrik T. Rasmussen** is a Scientific Fellow II at Vertex Pharmaceuticals Inc., in Cambridge, MA. He is currently responsible for the Analytical Development of several Phase I and Phase II compounds, including development of phase appropriate HPLC methods. He holds a B.S. in Chemistry (Magna Cum Laude) from Delaware Valley College of Science and Agriculture and a Ph.D. in Analytical Chemistry from Virginia Tech. His current research interests focus on means of improving accuracy, precision, and robustness of HPLC methods, on systematic approaches for achieving orthogonal chemical separations, and on the use of experimental designs and automation. He has (co-)authored over 20 publications and book chapters, has presented over 30 (invited) papers and posters at international symposia, and has taught numerous HPLC short courses. Dr. Rasmussen served as President of the 2003 Eastern Analytical Symposium and Exposition.

## Enhanced Productivity by Design in the Analytical Laboratory: Design of Experiments for Analytical Chemists

**One-Day Course E11-08, Sunday, November 13, 2011, 8:30am-5:30pm**

Dr. Zenaida Otero Gephardt, Rowan University, Glassboro, NJ

### COURSE DESCRIPTION

Experimentation in the analytical laboratory can be expensive and labor intensive. This is especially true for complex and highly regulated analyses. Optimization of experimental design techniques offers the advantage of minimizing the number of experiments required in the laboratory. This improves the efficiency of the laboratory staff and reduces the cost of operation. Experimental design techniques often yield better data, and results that are more meaningful and easier to interpret. Many design techniques are simple to use and only require a calculator or spreadsheet software. Experimental design techniques allow laboratory staff to focus on experimental development and to mainstream laboratory operations. This course will provide participants with analysis tools they can immediately use in their laboratories including an introduction to available experimental design software.

### WHO SHOULD ATTEND

Chemists and laboratory supervisors will benefit from this course. Researchers and technical personnel who design and carry out experiments will also benefit.

### TOPICS

Interactive exercises and practical examples will be used throughout the course.

- ▶ Background and Introduction to Experimental Design Optimization
- ▶ Simple Optimization Techniques and Applications
- ▶ Identifying Key Variables Using Optimization Techniques and Applications
- ▶ Optimization Techniques for Complex Systems and Applications
- ▶ Optimization Techniques for Experiments with Mixtures and Applications

### ABOUT THE INSTRUCTOR

**Dr. Zenaida Otero Gephardt** is Associate Professor of Chemical Engineering at Rowan University (Glassboro, NJ) and consultant through Otero Keil Associates. Her research focuses on optimization, development and mathematical modeling of chemical processes and laboratory techniques. She has developed statistical models and experimental designs for a wide range of chemical processes including high pressure, supercritical systems and multi-phase systems. Dr. Gephardt has worked with a wide range of system scales ranging from bench scale laboratory systems to large-scale industrial applications. Dr. Gephardt has over 20 years of experience with analysis and optimization applications in the chemical process industry. She teaches on-site courses for industry and provides analysis and experimental design support. Dr. Gephardt holds a Ph.D. in chemical engineering from the University of Delaware and is a registered Professional Engineer in Delaware.

## Impurity and Degradant Identification: Strategies for Structure Elucidation via Chromatography, MS and NMR

**MOne-Day Course E11-09, Sunday, November 13, 2011, 8:30am-5:30pm**

Dr. Thomas R. Sharp, Emeritus, Pfizer Global Research & Development, Groton, CT  
Dr. Brian L. Marquez, Pfizer Global Research and Development, Groton, CT  
Mr. Todd C. Zelesky, Pfizer Global Research and Development, Groton, CT

### COURSE DESCRIPTION

This course is designed to take participants through the process of impurity/degradant identification from start to finish. This course will be taught based on application driven materials and will only deal with very limited theory. This course will provide methods and approaches to solve a wide array of the impurity/degradation problems faced by structure elucidation scientists. The substrate provided will help guide individuals to solving more complex problems.

### WHO SHOULD ATTEND

This one-day course will benefit anyone interested in the practice of organic molecular structure determination. Focus and discussed examples will be on impurities and degradants found in pharmaceutical drug substances and products, but the principles are easily generalized.

### TOPICS

- ▶ Impurity/Degradant Isolation Techniques
  - Mass directed fraction collection
  - Supercritical fluid chromatography (SFC)
  - Trends in normal phase and reverse phase isolations
- ▶ MS and LC-MS
  - Historical perspective
  - Ionization methods and instrumentation
  - Accurate mass measurements
  - Clusters
  - Isotopes, isotopes, isotopes
  - Polymer patterns and multiply charged ions
  - Electrospray versus APCI
  - LC-MS-compatible buffers
  - MS-silent compounds
- ▶ NMR and LC-NMR
  - Basics of NMR and why it is an important tool for small molecule structure elucidation
  - Types of experiments used to solve particular problems
  - Utilization of hyphenation techniques: LC-NMR, LC-MS/NMR, other variations
  - Reaction NMR—monitoring real-time chemical reactions by NMR
- ▶ Example Problems
  - Case studies involving isolation, MS and NMR
  - Case studies involving more advanced NMR and MS techniques
  - Participants will discuss several case studies during this course

### ABOUT THE INSTRUCTORS

**Dr. Thomas R. Sharp** (Course Director) is an associate research fellow emeritus from Pfizer. He retired as a member of the research analytical co-discovery group in 2009. He previously headed a resource laboratory responsible to the division and the corporation focusing on the application of mass spectrometry to the structure elucidation of drug substance, impurity, and degradant molecules of interest to the company. He is now a member of the research analytical co-discovery group, providing early analytical chemical support to early development stage candidate molecules, which still includes impurity/degradant identification, as well as investigations into the computational chemistry aspects of molecule stability evaluation and expert systems development. He received his undergraduate degree in Zoology from Western Illinois University (1972), his Ph.D. from Indiana University (1977) in Biological Chemistry, has held postdoctoral appointments at Penn State University and Case Western Reserve University School of Medicine, fellowships from the American Cancer Society and the Muscular Dystrophy Association of America, and faculty/staff appointments at the University of Utah and Texas A&M University before joining Pfizer in 1991. Dr. Sharp received a Master's degree in Computer Science (1999) from Rensselaer Polytechnic Institute.

**Dr. Brian L. Marquez** is an associate research fellow at Pfizer Global Research and Development, Groton, CT. He currently leads the Structure Elucidation Group within the development organization. His team is responsible for the isolation and identification of unknown impurities and degradants from all stages of the drug development process. In addition, his group has the opportunity to explore and implement new advances in the fields of structure elucidation including NMR, MS, and isolation techniques. He received his undergraduate degree in Biochemistry and Biophysics from OregonStateUniversity (1997) and his Ph.D. from OregonStateUniversity (2001) in Medicinal Chemistry (Marine Natural Products Chemistry). Dr. Marquez has also held positions at Wyeth and Amgen doing structure elucidation by NMR spectroscopy.

**Mr. Todd C. Zelesky** is a scientist at Pfizer Global Research and Development, Groton CT. He currently works in the Structure Elucidation Group within the development organization. He is responsible for the isolation of impurities and degradants from all stages of the drug development process. He has explored and taken part in the implementation of technologies such as supercritical fluid chromatography that have impacted the isolation workflow and processes within the Structure Elucidation Group. He received his undergraduate degree in Chemistry at the University of Connecticut in 2000. Mr. Zelesky has also worked in The Forced Degradation Group as well as The Polymer Analysis and Characterization Group in Analytical Research and Development at Pfizer in Groton CT.

## **Impurities in Pharmaceuticals – A Survey Course**

**New One-Day Course E11-10, Sunday, November 13, 2011, 8:30am-5:30pm**

Dr. Bernard A. Olsen, Olsen Pharmaceutical Consulting, West Lafayette, IN

### COURSE DESCRIPTION

This course will provide information on a wide variety of impurities that may be present in small molecule drug substances and drug products. Each impurity topic will include a discussion of regulatory expectations, analytical considerations and method development, specifications, and strategies for addressing impurities throughout drug development. Specific topics to be covered include related substance process impurities, other synthetic process impurities, degradation products, excipient impurities and interaction products, stereochemical impurities, residual solvents, potentially genotoxic impurities, inorganic impurities, extractable and leachable impurities, and solid state forms.

### WHO SHOULD ATTEND

This one-day course will benefit chemists, engineers, formulation scientists, regulatory and quality personnel, and others in the pharmaceutical industry who would like to obtain a better background regarding issues involved with drug impurities and how to address them.

**TOPICS**

- ▶ Process Related Impurities in Drug Substances
  - ICH guidelines, impurity qualification, impurity reporting
  - Impurity origins, control, specifications
- ▶ Degradation Impurities in Drug Substances and Drug Products
  - ICH guidelines and specifications
  - Forced degradation studies
  - Excipient interactions
- ▶ Analytical Method Considerations for Impurity Investigation and Control
  - Screening methods
  - Control methods
- ▶ Chiral Purity
- ▶ Residual Solvents
- ▶ Genotoxic Impurities
  - Regulatory guidances
  - Assessment of impurities for genotoxicity
  - Analytical considerations for trace impurity determination
- ▶ Inorganic Impurities
- ▶ Extractables and Leachables
- ▶ Solid State Forms

**ABOUT THE INSTRUCTOR**

**Dr. Bernard A. Olsen** has over 29 years of experience at Eli Lilly and Company related to chemistry, manufacturing and control aspects of drug substances and drug products. He has contributed to the development and support of over 25 commercial drugs and numerous developmental drugs. He currently provides consulting services to the pharmaceutical industry and serves as Chair of the USP Expert Committee on Monograph Development-Small Molecules 3. He has published and given invited lectures on a wide array of drug development and analytical topics including high performance liquid chromatography, impurity determination and control, genotoxic impurities, physical property characterization, drug counterfeiting, regulatory aspects of drug development, and quality control. His undergraduate degree is from Nebraska Wesleyan University and his doctorate in analytical chemistry is from the University of Wisconsin-Madison. He is a Fellow of the American Association of Pharmaceutical Scientists.

**Polymers: An Introduction and Characterization and Techniques**

***New One-Day Course E11-11, Sunday, November 13, 2011, 8:30am-5:30pm***

Dr. Diep Nguyen, Illinois Institute of Technology, Chicago, IL

**COURSE DESCRIPTION**

Polymers have many applications in a variety of industries including the pharmaceutical industry, especially in coatings or in packaging of medicines; however, analysts working with polymer do not always have a formal training in the subject. This course is designed to give an introduction to polymeric materials and their potential uses. Participants will discuss various analytical methods to characterize polymers such as molecular weight determination, thermal analysis, determination of T<sub>g</sub> and rheology measurements.

**WHO SHOULD ATTEND**

This one-day course will benefit analysts, QA and QC managers, regulators, and researchers, who are not familiar with polymers and who would like to have an intensive introduction to polymers. Participants will gain a better understanding of polymers and a survey of polymer characterization techniques

**TOPICS**

- ▶ Polymer Nomenclature
- ▶ Molecular Weight and Molecular Weight Distribution
- ▶ Glass Transition Temperature
- ▶ Characterization Techniques: Molecular Weight, Thermal Properties, and Rheology
- ▶ Structure Property Relationships in Polymer

**ABOUT THE INSTRUCTOR**

**Dr. Diep Nguyen** is the Industry Professor at the Illinois Institute of Technology (IIT) in Chicago, IL. She is also the Director of the Professional Science Masters Program in Analytical Chemistry. After obtaining her Ph.D. in Polymer Chemistry from McGill University, Dr. Nguyen worked as a beamline scientist at the Brookhaven National Laboratories. She then joined PPG Company, working as a research chemist in the company's R&D center for seven years. Dr. Nguyen joined IIT in 2006, serving as the Director of the PSM program in Analytical Chemistry and as an Industry Professor.

Dr. Nguyen's research areas are in Polymer Characterization. Her publications and presentations cover a range of polymer characterization techniques. She has presented at the ACS national meeting about the PSM program and has been awarded the Excellent Teaching Award from the College of Science and Letters at IIT.

## How to Develop Validated HPLC Methods: Rational Design with Practical Statistics and Troubleshooting

**Two-Day Course E11-12, Monday and Tuesday, November 14 and 15, 2011, 8:30am-5:30pm**

Dr. Brian A. Bidlingmeyer, Agilent Technologies, Wilmington, DE

Dr. Stanley N. Deming, Statistical Designs, Houston, TX

### COURSE DESCRIPTION

This course offers practical training for the practicing scientist. This course takes the participant step-by-step through the concepts, techniques and tools necessary to develop validated HPLC methods. Learn a rapid, systematic approach to PLC methods development that provides sustainable validation by using statistical process control (SPC) tools. Rather than developing the HPLC method and then validating it, this course proposes following a streamlined, iterative process to integrate the method development and validation activities. The approach is effective, efficient and productive. The emphasis is on practical issues associated with developing validated HPLC methods. Case studies illustrate specific problems and how to approach them, how to carry out routine maintenance to prevent loss of validation, and how to set diagnostics to recognize behavior that requires troubleshooting. Discuss your specific method development/validation problems with instructors who have more than 60 years of combined experience in industry and academe. You will leave with a firm strategy for developing your own continually validated HPLC methods.

### WHO SHOULD ATTEND

This course is intended for individuals who will be or are developing and/or doing quantitative PLC analyses. Laboratory managers, supervisors, analysts, chemists, biologists, engineers and technicians who are responsible for the continual use of validated high-performance liquid chromatographic methods of chemical analysis should attend this course. Those working in R&D, manufacturing, QA/QC, methods development, process development, product testing, pharmaceuticals, biotechnology, organic chemicals, petroleum, environmental, foods, flavors, fragrances, pesticides, testing services laboratories, and occupational health and safety testing will all benefit from this course.

### TOPICS

- ▶ Method Evolution
  - Thinking ahead makes the tasks easier
  - The top four items to be successful
- ▶ Basic Statistical Concepts
  - Calculations with statistical significance
  - Parameters of merit
- ▶ Detection Options
  - Choices and trade-offs
  - Typical uses and sensitivities
- ▶ Determining Accuracy, Precision and Linearity
  - Making measurements
  - Proper calculation of validation parameters
- ▶ Achieving Separations
  - The chemistry of resolution
  - Follow the flow chart: a rational strategy for achieving resolution
- ▶ Sample Preparation
  - Review of techniques
  - How to improve the analysis
- ▶ Determining LOD, LOQ, MDL
  - Understanding your limits
  - A simple, fundamental statistical approach
- ▶ Achieving Method Stability and Robustness
  - System suitability
  - System component contributions
- ▶ Optimizing Using Window Diagrams
  - Finding the tallest trees in the forest
  - Choosing the best of several optima
- ▶ Using Statistical Quality Control of Separations
  - An easy graphical method
  - Achieving sustainable validation
- ▶ Troubleshooting Out-of-control Systems
  - Things you often forget to look for
  - Group discussion of typical issues
- ▶ Putting It All Together
  - Approaching the steps to validating a method
  - When steps are necessary and when they're not
- ▶ Case Studies

### ABOUT THE INSTRUCTORS

**Dr. Brian A. Bidlingmeyer** is employed by Agilent Technologies in Wilmington, DE. He is an accomplished separation scientist who has work experience in the chemical, pharmaceutical and instrumentation industries. He has published 2 books and more than 80 papers. Brian is the Chairman-elect of the Separations Science Subdivision of the American Chemical Society's Analytical Division and is active in the ASTM committee concerning chromatographic practices. He has made significant contributions to the practice and understanding of modern HPLC and has received numerous awards including the Heinrich Emmanual Merck Prize for contributions to analytical chemistry, the International Ion Chromatography Award for contributions to that area, and an IR 100 Award for a new method for amino acid analysis (Pico Tag Method). He is presently an associate editor of the *Journal of Chromatographic Science*.

**Dr. Stanley N. Deming** is Professor Emeritus at the University of Houston in Houston, TX. He is also the President of Statistical Designs, a firm that offers short courses and consulting in the areas of methods development, process optimization, statistical experimental design and the statistical analysis of laboratory data. He has taught (with Dr. Stephen L. Morgan) more than 500 highly acclaimed short

courses for the ACS and other organizations. He has co-authored 3 books and approximately 100 papers. He has been a member of the editorial boards of *Critical Reviews in Analytical Chemistry*, the *Journal of Chemometrics*, and *Chemometrics and Intelligent Laboratory Systems*.

## Putting Organic Chemistry into Perspective – A Review of Sophomore Organic Chemistry

**Two-Day Course E11-13, Monday and Tuesday, November 14 and 15, 2011, 8:30am-5:30pm**

Dr. John R. Sowa, Jr., SetonHallUniversity, South Orange, NJ

### COURSE DESCRIPTION

Putting Organic Chemistry into Perspective is a course that reviews the fundamentals of organic chemistry for analytical chemists. Often, the chemistry of organic compounds must be considered when choosing analytical strategies. We will review the essential tools needed for understanding organic chemistry and communicating with organic chemists.

### WHO SHOULD ATTEND

This is an organic chemistry course for analytical chemists. Analytical chemists dealing with organic compounds and communicating or working on projects with those who synthesize them will find this course very useful.

### TOPICS

- ▶ Acid-base Chemistry
- ▶ Functional Groups
- ▶ Nomenclature
- ▶ Structures of Pharmaceuticals
- ▶ Stereochemistry
- ▶ Fundamental Organic Reactions
- ▶ Principles of Organic Chemistry that are Relevant to Chromatography will also be Discussed

### ABOUT THE INSTRUCTOR

**Dr. John R. Sowa, Jr.**, is an associate professor at SetonHallUniversity. He received a B.S. from ManhattanCollege and a Ph.D. from IowaStateUniversity. He has taught an expanded version of this course at a local pharmaceutical company. His research interests include organic synthesis via homogeneous and heterogeneous catalysis, asymmetric synthesis and organoboron chemistry.

## Infrared Spectral Interpretation I & II

**Two-Day Course E11-14, Monday and Tuesday, November 14 and 15, 2011, 8:30am-5:30pm**

Dr. Brian C. Smith, Spectros Associates, Shrewsbury, MA

### COURSE DESCRIPTION

This course is a combination of two one-day courses: Infrared Spectral Interpretation I and Infrared Spectral Interpretation II courses. A discount will be offered for the combined course over separately registering for the two one-day courses. See course descriptions for Infrared Spectral Interpretation I and Infrared Spectral Interpretation II for details about the course.

### WHO SHOULD ATTEND

This course will benefit anyone who analyzes samples to determine chemical structures, and everyone for whom measuring infrared spectra is part of their job. Part I: Beginners will benefit from the introductory nature of this course. Experienced interpreters will benefit by learning systematic approaches to interpreting spectra and the review of spectra of important functional groups. Part II: All FTIR users will benefit by learning systematic approaches to interpreting spectra, the review of spectra of important functional groups, and how to use interpretation aids to make their job easier. Familiarity with the material in IR Spectral Interpretation I would be useful for attendees.

### TOPICS

#### **DAY ONE:**

See Topics listed under Infrared Spectral Interpretation I

#### **DAY TWO:**

See Topics listed under Infrared Spectral Interpretation II

### ABOUT THE INSTRUCTOR

See Instructor information under Infrared Spectral Interpretation single courses above.

## Infrared Spectral Interpretation I

**One-Day Course E11-15, Monday, November 14, 2011, 8:30am-5:30pm**

Dr. Brian C. Smith, Spectros Associates, Shrewsbury, MA

### COURSE DESCRIPTION

This is a one-day introduction to infrared spectral interpretation. You will learn how to integrate the peak position, height, and width information in a spectrum to successfully determine unknown molecular structures and to perform identities properly. The five ways of attacking mixture spectra are discussed, then a 12-step program to interpret spectra is presented. The diagnostic infrared bands of many economically important molecules including hydrocarbons, alcohols, ketones, esters, and polymers are presented. Attendees practice interpreting many unknown spectra in class with the instructor's guidance.

### WHO SHOULD ATTEND

This course will benefit anyone who analyzes samples to determine chemical structures, and everyone for whom measuring infrared spectra is part of their job. Beginners will benefit from the introductory nature of this course. Experienced interpreters will benefit by learning systematic approaches to interpreting spectra and the review of spectra of important functional groups.

### TOPICS

- ▶ The Fundamentals of Infrared Interpretation
  - The properties of light
  - Molecular vibrations
  - The meaning of peak positions, heights, and widths
  - A strategic approach to spectral interpretation
    - Dealing with mixtures
    - Performing identities properly
    - A systematic 12-Step approach to infrared interpretation
- ▶ Functional Group Analysis of Hydrocarbons
  - Alkanes: C-H stretching and bending vibrations
    - Straight chain alkanes
    - Estimating hydrocarbon chain length from IR spectra
  - Aromatic hydrocarbons
    - Mono-substituted benzene rings
    - Distinguishing ortho, meta, and para isomers
- ▶ Alcohols and Phenols
  - Differentiating primary, secondary, and tertiary alcohols
  - Phenols
  - Distinguishing alcohols from water
- ▶ The Carbonyl (C=O) Functional Group
  - Introduction to carbonyl spectra
  - Ketones
  - Esters: the rule of 3
  - Summary
- ▶ Introduction to the Infrared Spectra of Polymers
  - Low- and high-density polyethylene
  - Polypropylene
  - Polystyrene
  - Polyethylene Terephthalate (PET)

### ABOUT THE INSTRUCTOR

**Dr. Brian C. Smith** is founder and principal of Spectros Associates. He has been a spectroscopist for over 30 years and was employed by Bell Labs and Digilab. He is an experienced trainer; thousands of people have benefited from his instruction as part of Spectros Associates since 1992. Dr. Smith is the author of three popular books on spectroscopy; *Fundamentals of FTIR* and *Infrared Spectral Interpretation* published by CRC Press, and *Quantitative Spectroscopy: Theory and Practice* published by Academic Press. Dr. Smith earned his Ph.D. in Chemistry from Dartmouth College and graduated with highest honors from Rochester Institute of Technology with a B.S. in Chemistry.

## Critical cGMP and ICH Guidances for Analytical Laboratories

**One-Day Course E11-16, Monday, November 14, 2011, 8:30am-5:30pm**

Ms. Kim Huynh-Ba, United States Pharmacopeia, Newark, DE  
Dr. Linda L. Ng, US Food and Drug Administration, Silver Spring, MD

### COURSE DESCRIPTION

Analytical laboratories hold major functions in the pharmaceutical industry. Throughout this course, critical cGMPs regulations, FDA guidances and ICH Quality guidelines will be introduced specifically emphasizing procedures to help individuals to comprehend the management aspects of the laboratory in order to maintain a high level of compliance that surrounds the laboratory environment. It also reviews several quality systems that support the analytical laboratory such as:

- cGMP regulations
- Analyst Training Program
- Controls of Standards and Samples
- Laboratory Records and Reports
- Analytical Method Validation
- Equipment Calibration and Qualification
- Stability Program
- Laboratory Investigation

### WHO SHOULD ATTEND

This one-day course will benefit analysts and researchers, who perform analytical testing in analytical laboratory for pharmaceutical analyses. It will introduce individuals to cGMP and ICH and FDA regulations that cover the quality systems, controls and operations of the laboratory functions. It is intended for manufacturers of OTC, generics and new drug products as well as contract research organizations (CROs), government labs since the pharmaceutical products have similar regulatory requirements.

To get the most out of the course, we highly recommended that you have at least two years of pharmaceutical analysis or drug development experience.

### TOPICS

- ▶ Laboratory Control and the Drug Development Process
- ▶ ICH and Related ICH Quality Guidances
- ▶ Method Validation
- ▶ Stability Program and Related Topics
- ▶ CMC Documentation: Records and Reports

### ABOUT THE INSTRUCTORS

**Kim Huynh-Ba** is the Director of Pharmacopeial Education Department of US Pharmacopeia. She has twenty two years of experience in various analytical areas of pharmaceutical development and a primary focus in stability sciences. Prior to USP, she held positions in drug development at Astra Zeneca (formerly ICI Americas), DuPont Merck, DuPont Pharmaceuticals, Bristol Myers Squibb and Wyeth Vaccines. Since 2002 to 2011, she has been advising pharmaceutical companies including companies operating under Consent Decree on harmonization and optimization of analytical best practices as the Technical Director at Pharmalytik Consulting Services. Kim is also a short course instructor and organizer on topics ranging from cGMP compliance and quality issues to stability programs under sponsorship of global organizations such as American Chemical Society (ACS), American Association of Pharmaceutical Scientists (AAPS), Pittsburgh Conference, many other international training groups. She is an adjunct professor at Temple University, School of Pharmacy and Illinois Institute of Technology. She also received the 2001 DPCAA Leadership Award.

Kim Huynh-Ba has authored numerous technical publications and book chapters. She is invited frequently to present at national and international conferences. She is the editor of the *"Handbook of Stability Testing in Pharmaceutical Development: Regulations, Methodologies and Best Practices"* (ISBN: 978-0387856261), and also *"Pharmaceutical Stability Testing to Support Global Markets"* (ISBN: 978-1-4419-0888-9).

**Dr. Linda L. Ng** is currently the Chemistry Manufacturing and Controls (CMC) Lead for Ophthalmology, Office of New Drug Quality Assessment (previously the Chemistry Team Leader), Center for Drug Evaluation and Research, Food and Drug Administration in Silver Spring, Maryland. She served as the CDER Chair of the Analytical Methods Technical Committee; drafted the CDER Reviewer Guidance: Validation of Chromatographic Methods; and was the FDA Topic Leader for the ICH Q2 Guidance. She has been invited to present and publish nationally and internationally in the area of method validation.

Dr. Ng is serving as the President of the Sigma Xi FDA Chapter, and was on the USP Expert Committee on Pharmaceutical Analysis 6, 2005-2010. She was the Vice Chair of the USP Expert Committee on Pharmaceutical Analysis 2 (2000-2005), and Chair of the USP working group on Column Classification. For the AOAC International, she served as the Chair of the Peer-Verified Methods Advisory Committee; member of the Task Force on Integration of the Methods Validation Programs; member, General and Associate Referees of the Committee for Drugs and Related Topics; and Associate Chapter Editor of the Official Methods of Analysis. She obtained her undergraduate degree from Western College, her Ph.D. from the University of Illinois, Champaign-Urbana, and had post-doctoral training at the Massachusetts Institute of Technology. She spent ten years in the pharmaceutical industry before joining FDA as a Review Chemist and later as an Expert Review Chemist.

## **Physical Characterization and Analytical Test of Pharmaceutical Solids II: Advanced Applications**

**One-Day Course E11-17, Monday, November 14, 2011, 8:30am-5:30pm**

Dr. Steve R. Byrn, Purdue University, West Lafayette, IN  
Dr. Xiaoming (Sean) Chen, OSI Pharmaceuticals, Inc, Cedar Knolls, NJ

### COURSE DESCRIPTION

Physical characterization and methods of analysis of pharmaceutical solids are widely applied in drug research and development. Drug substances are generally manufactured as solid-state forms and drug products are typically marketed as solid dosage formulations. Qualitative and quantitative analysis using various solid state methods are necessary for ensuring the quality and stability of drug substances and products. This short course offers some advanced concepts for pharmaceutical analysis including a review of particle size/surface area, hydration/dehydration, and physical stability/physical transformation. It also discusses important applications of analytical methods of pharmaceutical solids in form selection, mixture analysis, solid dispersions, and nanotechnology.

### WHO SHOULD ATTEND

This one-day course will benefit formulation scientists, process engineers, analysts, QA and QC managers, regulators, and researchers, who perform process development and manufacture of drug substances, develop formulations of drug products, conduct analytical testing and method development, set up stability programs, and evaluate stability data of drug substances and products.

### TOPICS

- ▶ Pharmaceutical Solids—Advanced Concepts
  - Particle size/surface area
  - Water sorption, hydration/dehydration
  - Physical stability/physical transformation
- ▶ Important Applications
  - Form selection
  - Mixture analysis
  - Solid dispersions
  - Nanotechnology

### ABOUT THE INSTRUCTORS

**Dr. Stephen R. Byrn** is Charles B. Jordan Professor of Medicinal Chemistry in the School of Pharmacy, Purdue University, West Lafayette, Indiana. He is also Head of the Department of Industrial and Physical Pharmacy. He received his B.A. degree in Chemistry from DePauw University and his Ph.D. degree in Chemistry from the University of Illinois, Urbana. He did postdoctoral research at UCLA. His research focuses on solid state chemistry, polymorphism, stability, manufacturing science, quality by design, and medicinal chemistry. Dr. Byrn opened up the field of solid state chemistry of drugs with his research and books of that title (first edition, 1982, second edition, 2000). Dr. Byrn has founded and directed several programs at Purdue University including CAMP, the Center for AIDS Research, the Molecules to Market program, and Purdue's graduate programs in regulatory and quality compliance. He is also one of the founders and a member of the executive committee of NIPTE (National Institute for Pharmaceutical Technology and Education). He continues to be involved in educating scientists in solid state chemistry, methods of analysis, and regulatory science. Dr. Byrn has served as chair of the Pharmaceutical Sciences Advisory Committee to the FDA and Chair of the Drug Substances Technical Committee, Product Quality Research Initiative. Dr. Byrn has extensive experience as a consultant in the pharmaceutical industry and currently serves as Purdue's representative to the USP. Dr. Byrn is co-founder of SSCI, Inc. (Solid State Chemical Information) a cGMP research and information Company specializing in polymorphism, crystallization, analysis, problem solving and regulatory issues. SSCI, Inc. is now owned by Aptuit and Dr. Byrn serves as Head of the Aptuit Scientific Advisory Board. Dr. Byrn is also a technical founder of Andara now owned by Cyberkinetics, Inc. Andara specializes in devices and drugs for the treatment of spinal cord injury and CNS diseases.

**Dr. Xiaoming (Sean) Chen** received his Ph.D. in Industrial and Physical Pharmacy from Purdue University in 2000. He has worked as a project leader in discovery support and preformulation at Schering-Plough Research Institute for five years. He has contributed the nomination of five NCE for development and received one President Award, one Impact Award and Three Excellence Awards from Schering-Plough Research Institute. He has also worked in Exploratory Formulation group of Schering-Plough for three years, leading formulation development of two important line extension projects. Currently, Dr. Chen is a Senior Development Investigator in Pharmaceutical Development of OSI Pharmaceuticals. Dr. Chen is an expert in physical characterization of solids, crystal form and salt selection, and controlled release formulation. He has published over a dozen of papers in peer-reviewed journals. Dr. Chen is a member of AAPS and has served in PDD award committee for two years.

## **Analytical Laboratory Techniques for Analytical Laboratory Staff**

**One-Day Course E11-18, Monday, November 14, 2011, 8:30am-5:30pm**

Dr. Merlin K. L. Bicking, ACCTA, Inc., St. Paul, MN

### COURSE DESCRIPTION

Good technique is essential in every successful analytical laboratory. *However, laboratory analysts in many industries (e.g., pharmaceutical, medical device, etc.)* have particularly challenging job requirements, due to both regulatory (e.g., GMP and GLP) and economic demands. This seminar can help your entire laboratory realize better efficiency and data quality, by ensuring that every staff member has the same basic level of training. Based on discussions with analytical scientists in these industries, this seminar provides a broad range of topics that are directly related to the laboratory activities of the typical analyst. Rather than simply demonstrating a particular procedure, the course provides some background information about common laboratory techniques, along with the “do’s and don’ts”, so that the analysts have a better perspective about why they must perform these tasks in a certain way

### WHO SHOULD ATTEND

This one-day course will benefit

- New laboratory staff - either recent graduates or transfers from other groups
- Specialists who want to add new skills or need cross-training instruction
- Experienced analysts and technicians who want or need a brief refresher course
- Anyone needing the “education, training, and experience, or any combination thereof ...” to work in a GMP environment.

### TOPICS

- ▶ Mathematical Skills: A Review of Basic Calculation Principles
  - Perspectives
  - Units, units conversions, and calculations
  - Chemical factors
  - Significant figures and rounding
  - Method-related calculations
- ▶ Using Laboratory Equipment: Avoiding the Most Common Problems
  - Analytical balances
  - pH meters
  - Filtration
- ▶ Volumetric Containers: Why We Do What We Do
  - General issues with volumetric glassware
  - Specifications and calibration
  - Volumetric flasks and pipets
  - Pipetting instruments (Pipettors)
- ▶ Solution Preparation Issues: Putting it All Together
  - Propagation of errors
  - Preparation of solutions and standards
  - Documentation and observation

### ABOUT THE INSTRUCTOR

**Dr. Merlin K. L. Bicking**, President, *ACCTA, Inc.* He has extensive analytical chemistry experience in academia, contract research, independent testing laboratories, consulting, and technical training. His professional history includes development of two EPA methods, as well as numerous methods in other regulated and non-regulated industries. His publications and presentations cover a wide range of topics, including liquid chromatography theory, derivatization, method optimization, and the use of experimental design strategies in analytical chemistry. He also develops and presents technical training seminars for analytical laboratory staff.

## Laboratory Data Analysis Using EXCEL®: New Uses for a Familiar Tool

**One-Day Course E11-19. Monday, November 14, 2011, 8:30am-5:30pm**

Dr. Zenaida Otero Gephardt, RowanUniversity, Glassboro, NJ

### COURSE DESCRIPTION

This course focuses on the features of EXCEL® that can be used by experimenters and researchers to analyze their data in a simple and straightforward manner. EXCEL® can be a powerful tool in the analytical chemist's data analysis tool box. EXCEL® is widely available and can serve to enhance the quality and effectiveness of data analysis and laboratory operations. A wide range of laboratory data analysis applications will be discussed. Participants will be able to immediately use the material covered in the course to enhance their effectiveness in the laboratory.

### WHO SHOULD ATTEND

Analytical chemists at all levels will benefit from this course. Laboratory supervisors and technical personnel involved in data analysis and reporting will also benefit.

### TOPICS

Interactive exercises and practical examples will be used throughout the course.

- ▶ Introduction and the Basics of EXCEL®
- ▶ Spreadsheet Development and Manipulation
- ▶ Data Analysis Techniques
  - Assessment of data quality
  - Graphical and numerical analysis methods
  - Linear regression
  - Non-linear regression using the solver
- ▶ Custom Applications

### ABOUT THE INSTRUCTOR

**Dr. Zenaida Otero Gephardt** is Associate Professor of Chemical Engineering at RowanUniversity (Glassboro, NJ) and consultant through Otero Keil Associates. Her research focuses on optimization, development and mathematical modeling of chemical processes and laboratory techniques. She has developed statistical models and experimental designs for a wide range of chemical processes including high pressure, supercritical systems and multi-phase systems. Dr. Gephardt has worked with a wide range of system scales ranging from bench scale laboratory systems to large-scale industrial applications. Dr. Gephardt has over 20 years of experience with analysis and optimization applications in the chemical process industry. She teaches on-site courses for industry and provides analysis and experimental design support. Dr. Gephardt holds a Ph.D. in chemical engineering from the University of Delaware and is a registered Professional Engineer in Delaware.

## Concepts in Sustainability and Green Chemistry

**New One-Day Course E11-20, Monday, November 14, 2011, 8:30am-5:30pm**

Dr. Douglas E. Raynie, South Dakota State University, SD

### COURSE DESCRIPTION

This short course is designed to provide participants with an understanding of the principles of sustainability and green chemistry. Upon successful completion of the course, the participant will have an understanding of the principles of green chemistry, the principles of green engineering, and resources to further their understanding of green chemistry. The course will begin by discussing principles of green chemistry and engineering as a supporting pillar of sustainable development. Case studies will be presented to exemplify each of these green chemistry principles. Finally, green chemistry education and resources will be presented. Throughout the course both principles and practical aspects of the outlined topics will be presented.

### WHO SHOULD ATTEND

This one-day course will benefit lab managers, technicians and others involved in developing analytical or chemical methods

### TOPICS

- ▶ Introduction
  - Sustainability
  - The principles of Green Chemistry
  - The principles of Green Engineering
- ▶ Case Studies
  - Waste
  - Life cycle assessment
  - Safer solvents
  - Renewable feedstocks
  - Crystal Faraday Partnership
- ▶ Green Analytical Chemistry
  - Approaches
  - Greenness profile
- ▶ Green Chemistry Education
  - ▶ Resources
    - Green Chemistry Institute
    - Books and printed resources
    - Web-based resources
    - Universities and research opportunities
  - ▶ Summary
    - Current state of the field
    - Challenges

### ABOUT THE INSTRUCTOR

**Dr. Douglas E. Raynie** is a Research Assistant Professor in the Department of Chemistry and Biochemistry at South Dakota State University. Prior to joining SDSU, he was employed for eleven years as a Senior Scientist at Procter and Gamble's Corporate Research Division. He earned his Ph.D. at Brigham Young University under the direction of Dr. Milton L. Lee. His undergraduate degree is from Augustana (South Dakota) College, with majors in chemistry and biology. Analytical separations research in Dr. Raynie's laboratory includes high-resolution chromatography (high-temperature LC and SFC), chromatographic sample preparation (ASE, SFE, SPME, and SPE), chromatography theory, green analytical chemistry, and problem-based learning in analytical chemistry.

## The Analysis and Characterization of Protein Therapeutic Drugs

**Two-Day Course E11-21, Tuesday and Wednesday, November 15 and 16, 2011, 8:30am-5:30pm**

Mr. C. David Carr, Bioanalytical Technologies, Wrightwood, CA

### COURSE DESCRIPTION

Explanations of the properties of proteins that must be characterized in the course of developing a protein therapeutic drug and monitored during production and lot release begin this class. The theory and practice of a number of chromatographic separation techniques that play key roles in the analysis and characterization of protein therapeutic drugs are then described during the first day of the class. The chromatography techniques that are discussed include reversed-phase HPLC, ion exchange, size exclusion and several less well-known techniques in chromatography. Examples of how these are used in the development and release of protein therapeutic drugs are shown. (Note: The first day is the same as the class: The Role of Chromatography in the Analysis and Characterization of Protein Therapeutic Drugs.) The second day of the class explains and discusses Capillary Electrophoresis and Mass Spectrometry and reviews their respective roles in protein drug analysis and characterization. The purposes of these two techniques in protein drug analysis are discussed and examples are shown.

### WHO SHOULD ATTEND

This course is designed for young scientists embarking on a career in biotechnology analysis as well as experienced scientists starting to work with the analysis of protein therapeutic drugs. Attendees may have degrees in chemistry, biology or related fields. It is suitable for those in quality control, quality assurance, research and development and production monitoring.

**TOPICS**

- ▶ Protein Properties Relevant to the Therapeutic Properties of Protein Drugs
  - Deamidation
  - Oxidation
  - Glycosylation
  - Charge state variants
  - Aggregation and denaturation
  - Pegylation and other forms of conjugation
- ▶ Reversed-Phase HPLC and its Role in Protein Therapeutic Analysis
  - Typical operating conditions for protein/peptide analysis
  - Column characteristics best suited for protein and peptide analysis
  - Optimum mobile phase conditions
  - The effect of gradients and temperature on peptide separations
- ▶ How Reversed-phase HPLC is used to Characterize and Analyze Protein Therapeutics for Degradation Products, Disulfide Bonds, Glycosylation, and other Modifications
- ▶ Other Types of Liquid Chromatography and their Respective Roles in Protein Therapeutic Drug Analysis
  - Ion Exchange chromatography
  - High pH Anion Exchange Chromatography
  - Normal Phase Liquid Chromatography
- Hydrophobic Interaction Chromatography
- Size Exclusion Liquid Chromatography
- ▶ The Essential Theory and Practice of Capillary Electrophoresis
  - Mobility, migration, electroosmotic flow, joule heating
  - Instrument considerations: detection, injection
  - Operating conditions for Capillary Zone Electrophoresis (CZE)
  - Examples of how CZE is used in protein drug analysis
  - Capillary isoelectric focusing electrophoresis: operating conditions and uses in protein analysis and characterization
  - Capillary gel electrophoresis: operating conditions and uses in protein drug analysis
- ▶ Mass Spectrometry as used in Protein Drug Analysis
  - Description of ion sources: electrospray and Matrix-assisted Laser Desorption (MALDI)
  - Description of commonly used mass analyzers including the quadrupole, ion trap and time of flight (TOF)
  - Operating parameters and characteristics of LC-MS
  - The use of mass spectrometry to monitor molecular weights of protein drug products and how this information is useful in identifying and monitoring protein modifications.
  - Peptide fragmentation and its role in protein drug characterization.

**ABOUT THE INSTRUCTOR**

**Mr. C. David Carr** graduated from the University of California, Berkeley, with a degree in chemistry and did graduate work in molecular biology at the University of California, San Diego. He has been involved in High-Performance Liquid Chromatography for nearly forty years. He has worked with the biotechnology industry for many years in the characterization and analysis of protein therapeutics. He is the author of the popular booklet *"The Handbook of Analysis and Purification of Proteins and Peptides by Reversed-Phase HPLC"* and is very experienced with the uses of chromatography, electrophoresis and mass spectrometry for the analysis of proteins and peptides. For the past ten years he has been the principal instructor for Bioanalytical Technologies ([www.bioanalyticaltech.com](http://www.bioanalyticaltech.com)), teaching classes on the Analysis and Characterization of Protein Therapeutic Drugs. He has taught this class to scientists from most of the major biotechnology firms such as Amgen, Genentech, Biogen Idec and Genzyme as well as members of the staff of a great many smaller biotech companies.

## The Role of Chromatography in the Analysis and Characterization of Protein Therapeutic Drugs

**One-Day Course E11-22, Tuesday, November 15, 2011, 8:30am-5:30pm**

Mr. C. David Carr, Bioanalytical Technologies, Wrightwood, CA

**COURSE DESCRIPTION**

Explanations of the properties of proteins that must be characterized in the course of developing a protein therapeutic drug and monitored during production and lot release begin this class. The theory and practice of a number of chromatographic separation techniques that play key roles in the analysis and characterization of protein therapeutic drugs are then described. The chromatography techniques that are discussed include reversed-phase HPLC, ion exchange, size exclusion and several less well-known techniques in chromatography. Examples of how these are used in the development and release of protein therapeutic drugs are shown.

**WHO SHOULD ATTEND**

This course is designed for young scientists embarking on a career in biotechnology analysis as well as experienced scientists starting to work with the analysis of protein therapeutic drugs. Attendees may have degrees in chemistry, biology or related fields. It is suitable for those in quality control, quality assurance, research and development and production monitoring.

**TOPICS**

- ▶ Protein Properties Relevant to the Therapeutic Properties of Protein Drugs
  - Deamidation
  - Oxidation
  - Glycosylation
  - Charge state variants

- Aggregation and denaturation
- Pegylation and other forms of conjugation
- ▶ Reversed-Phase HPLC and its Role in Protein Therapeutic Analysis
  - Typical operating conditions for protein/peptide analysis
  - Column characteristics best suited for protein and peptide analysis
  - Optimum mobile phase conditions
  - The effect of gradients and temperature on peptide separation
- ▶ How Reversed-phase HPLC is used to Characterize and Analyze Protein Therapeutics for Degradation Products, Disulfide Bonds, Glycosylation, and other Modifications
- ▶ Other Types of Liquid Chromatography and their Respective Roles in Protein Therapeutic Drug Analysis
  - Ion Exchange chromatography
  - High pH Anion Exchange Chromatography
  - Normal Phase Liquid Chromatography
  - Hydrophobic Interaction Chromatography
  - Size Exclusion Liquid Chromatography

#### **ABOUT THE INSTRUCTOR**

**Mr. C. David Carr** graduated from the University of California, Berkeley, with a degree in chemistry and did graduate work in molecular biology at the University of California, San Diego. He has been involved in High-Performance Liquid Chromatography for nearly forty years. He has worked with the biotechnology industry for many years in the characterization and analysis of protein therapeutics. He is the author of the popular booklet *"The Handbook of Analysis and Purification of Proteins and Peptides by Reversed-Phase HPLC"* and is very experienced with the uses of chromatography, electrophoresis and mass spectrometry for the analysis of proteins and peptides. For the past ten years he has been the principal instructor for Bioanalytical Technologies ([www.bioanalyticaltech.com](http://www.bioanalyticaltech.com)), teaching classes on the Analysis and Characterization of Protein Therapeutic Drugs. He has taught this class to scientists from most of the major biotechnology firms such as Amgen, Genentech, Biogen Idec and Genzyme as well as members of the staff of a great many smaller biotech companies.

## **Infrared Spectral Interpretation II**

**One-Day Course E11-23, Tuesday, November 15, 2011, 8:30am-5:30pm**

Dr. Brian C. Smith, Spectros Associates, Shrewsbury, MA

#### **COURSE DESCRIPTION**

A more detailed look at infrared interpretation for anyone who needs to identify unknown molecules using infrared spectroscopy. Learn how molecules absorb infrared light so you can fully understand all the features in a spectrum. The spectra of economically important but spectrally complex molecules are explained using many examples. Discover how spectral subtraction and library searching can make interpreting spectra easier. Attendees practice interpreting many unknown spectra in class with the instructor's guidance.

#### **WHO SHOULD ATTEND**

This course will benefit anyone who analyzes samples to determine chemical structures, and everyone for whom measuring infrared spectra is part of their job. All FTIR users will benefit by learning systematic approaches to interpreting spectra, the review of spectra of important functional groups, and how to use interpretation aids to make their job easier. Familiarity with the material in IR Spectral Interpretation I would be useful for attendees.

#### **TOPICS**

- ▶ How Molecules Absorb Infrared Radiation
  - How molecules absorb infrared light
  - Assigning all the features in a spectrum
- ▶ Unsaturated Hydrocarbons
  - Alkenes:
    - Substitution patterns
    - Distinguishing Cis/Trans Isomers
    - Natural and synthetic rubbers
  - Alkynes
- ▶ Ethers
  - Saturated Ethers
  - Aromatic Ethers
  - The Methoxy Group
- ▶ Complex Carbonyl Molecules
  - Aldehydes
  - Carboxylic Acids
  - Carboxylates (Soaps)
- ▶ Organic Nitrogen Compounds
  - Amides
    - Structure, nomenclature, and bonding
  - Primary Amides
  - Secondary Amides
  - Proteins
  - Amines
    - Distinguishing the three types of amines
    - Methyl groups bonded to Nitrogen
    - Amine Salts
    - Nitriles
    - The Nitro Group
- ▶ Interpretation Aids
  - Spectral subtraction: simplifying mixture spectra
    - Theory
    - Optimizing subtraction results
    - Spotting artifacts
  - Library searching
    - Background and theory
    - The search process
    - Properly interpreting search results
    - Subtract and search again: deconstructing mixtures

**ABOUT THE INSTRUCTOR**

**Dr. Brian C. Smith** is founder and principal of Spectros Associates. He has been a spectroscopist for over 30 years and was employed by Bell Labs and Digilab. He is an experienced trainer; thousands of people have benefited from his instruction as part of Spectros Associates since 1992. Dr. Smith is the author of three popular books on spectroscopy; *Fundamentals of FTIR* and *Infrared Spectral Interpretation* published by CRC Press, and *Quantitative Spectroscopy: Theory and Practice* published by Academic Press. Dr. Smith earned his Ph.D. in Chemistry from Dartmouth College and graduated with highest honors from Rochester Institute of Technology with a B.S. in Chemistry.

**Sample Preparation: The Chemistry Behind the Techniques****One-Day Course E11-24, Tuesday, November 15, 2011, 8:30am-5:30pm**

Dr. Douglas E. Raynie, South Dakota State University, SD  
 Dr. Merlin K. L. Bicking, ACCTA, Inc., Woodbury, MN

**COURSE DESCRIPTION**

Come prepared to learn that sample preparation is more than just a few “low tech” procedures. Learn about the chemical principles behind the techniques, and how an understanding of these principles will produce better results in your laboratory. This course will include a survey of many traditional procedures, including information on recent advances in these techniques. Several new sample preparation technologies will also be introduced.

This is not a “recipe” course limited to a particular sample type or application. This course offers a comprehensive treatment of sample preparation as an important part of every analytical method. You will learn more than just a few manipulations; you will come away with a complete understanding of what sample preparation is and how you can use it!

This has been a popular course at EAS for many years, and has been updated to provide you with a good understanding of modern sample preparation.

**WHO SHOULD ATTEND**

Analytical chemists from all areas, especially those who want to learn more about sample preparation techniques, including preparation laboratory staff, analysts, and supervisors, will benefit from this course.

**TOPICS**

- ▶ Perspectives on the Importance of Sample Preparation
- ▶ General Principles Used in Sample Preparation Procedures
  - Physical changes, LeChatelier’s Principle
  - Effects of temperature, time, ionic strength, and pH
  - Like-dissolves-like
  - Two-phase partitioning equilibria
- ▶ Traditional Laboratory Procedures
  - Filtration
  - Solvent evaporation
  - Solvent exchange
- ▶ Traditional Laboratory Techniques
  - Derivatization
  - Liquid-liquid extraction (techniques, variations, and recent advances)
  - Liquid-solid extraction (traditional technologies and recent advances)
  - Solid phase extraction (SPE)
  - Membrane disk extractions
- ▶ “New” Sample Preparation Technologies
  - GC sample preparation (headspace, thermal desorption)
  - Supercritical fluid extraction (SFE)
  - Solid phase micro extraction (SPME)
  - Accelerated solvent extraction (ASE)
  - Other new ideas (SBSE and others)

**ABOUT THE INSTRUCTORS**

**Dr. Douglas E. Raynie** (Course Director) is a Research Assistant Professor in the Department of Chemistry and Biochemistry at South Dakota State University. Prior to joining SDSU, he was employed for eleven years as a Senior Scientist at Procter and Gamble’s Corporate Research Division. He earned his Ph.D. at Brigham Young University under the direction of Dr. Milton L. Lee. His undergraduate degree is from Augustana (South Dakota) College, with majors in chemistry and biology. Analytical separations research in Dr. Raynie’s laboratory includes high-resolution chromatography (high-temperature LC and SFC), chromatographic sample preparation (ASE, SFE, SPME, and SPE), chromatography theory, green analytical chemistry, and problem-based learning in analytical chemistry.

**Dr. Merlin K. L. Bicking** is President, ACCTA, Inc. He has extensive analytical chemistry experience in academia, contract research, independent testing laboratories, consulting, and technical training. His professional history includes development of two EPA methods, as well as numerous methods in other regulated and non-regulated industries. His publications and presentations cover a wide range of topics, including liquid chromatography theory, derivatization, method optimization, and the use of experimental design strategies in analytical chemistry. He also develops and presents technical training seminars for analytical laboratory staff.

## Introduction to Near-Infrared Spectroscopy: Applications in the Pharmaceutical and Biotech Industries

**IndustrieOne-Day Course E11-25, Tuesday, November 15, 2011, 8:30am-5:30pm**

Dr. Emil Ciurczak, Doramaxx Consulting, Goldens Bridge, NY

### COURSE DESCRIPTION

Near-Infrared Spectroscopy (NIRS) is a non-destructive, rapid method for determining both chemical and physical properties of pure materials (API and excipients), packaging materials, mixtures, solutions, and solid dosage forms. This course will review the theory and equipment used in NIR, the most common software packages, and some qualitative and quantitative applications.

### WHO SHOULD ATTEND

This course is a good introduction to analysts, lab managers, QA/QC personnel, and any person involved with process analysis (PAT/QbD). The course will benefit anyone considering NIR as a tool as well as analysts already performing NIR analyses. Attendees need not be a spectroscopist to benefit from the course.

### TOPICS

- ▶ Basic Theory and History
  - A brief history and theory
  - Why NIR is different from “classic” spectrometric methods
  - What can be seen and where NIR may not be best applied
- ▶ Some Hardware Available
  - Interference and linear variable filters
  - Gratings
  - Interferometers
  - Acousto-Optic tunable filters
  - Strengths and weaknesses of each, and where each would be best applied
- ▶ Software and Chemometrics
  - Multiple linear regression (MLR)
  - Principal components analysis (PCA)
  - Partial least squares (PLS)
- Mahalanobis Distances, Conformity Index, Spectral Matching
- Some 3<sup>rd</sup> party software available
- ▶ Qualitative Applications
  - Raw material ID/qualification (RMID)
  - Clinical trials/counterfeiting
  - Polymorphic changes
  - Fermentation reaction ingredients
- ▶ Quantitative Applications
  - Moisture (RM, drying, Lyophilization)
  - % polymorph and % crystallinity
  - Assay
  - Content uniformity
  - Process monitoring
- ▶ Validation of Equations (FDA, ICH, EMA)

### RECOMMENDED TEXT

Recommended Text: “Handbook of Near-Infrared Analysis”, 3rd Edition, Burns and Ciurczak, eds., CRC Press, 2007

### ABOUT THE INSTRUCTOR

**Dr. Emil Ciurczak** has degrees in chemistry from Rutgers and SetonHallUniversities and worked in the Pharma industry since 1970 at Ciba-Geigy, Cooper Labs (Berlex), Sandoz, Merck, and Purdue Pharma. He has also worked with or consulted for Technicon (Bran+Leubbe), FOSS NIRSystems, Brimrose, Infrared Fiber Systems, and Control Development. Emil introduced NIR at Sandoz in 1983 and was checking all raw materials (100% container-wise testing) by 1985.

He is now President of Doramaxx Consulting, performing NIR, PAT and QbD applications and teaching courses in PAT and NIR in the US and Europe; he was the 2004 recipient of the EAS NIR Award. Emil holds nine patents for NIR equipment and software.

Emil is co-author of “The Handbook of NIR Analysis” (3 editions) and “Medical and Pharmaceutical Applications of NIR.” He was a contributing editor to Spectroscopy from 1988 to 2005, and is presently Contributing Editor for *Pharmaceutical Manufacturing* magazine. He has published over 75 papers and has over 150 presented papers.

## How to Create a More Effective Lab Safety Program

**One-Day Course E11-26, Tuesday, November 15, 2011, 8:30am-5:30pm**

Dr. James A. Kaufman, Laboratory Safety Institute, Natick, MA

### COURSE DESCRIPTION

Safety in The Laboratory is an intensive one-day program designed to review the fundamentals of lab safety and assist scientists and science educators in the development and improvement of their lab safety program.

Participants discuss important lab safety problems and find solutions for many of them. The course emphasizes the need to make health, safety, and the environment an integral and important part of education, work and life. You'll learn dozens of ways to convince others that lab safety is important (and that you're serious about it).

This course is based on "Prudent Practices, the OSHA Lab Standard, ANSI Standards, NFPA Standards, and recognized professional standards from the American Chemical Society, the American Association of Physics Teachers, NIC, ASM, and the CDC.

Learn new presentation techniques and methods for conveying the importance of lab safety to your colleagues. Learn how to comply with many OSHA, EPA, and DOT requirements that impact Laboratories.

### **WHO SHOULD ATTEND**

Lab Managers, lab workers, lab technicians, analytical chemists, lab supervisors, group leaders, principal investigators, researchers, science and engineering faculty and staff, clinical and forensic scientists, and anyone who would like to have and improved lab safety program, reduce the likelihood of injury, illness, regulatory violation fines, and negligence lawsuits.

### **TOPICS**

- ▶ Introduction
- ▶ Three C's of Safety
- ▶ Scope of the Problem
- ▶ Accidents
- ▶ Legal Aspects
- ▶ Emergency Planning
- ▶ Handling and Storing Chemicals
- ▶ Biological and Animal Hazards
- ▶ Eye and Fact Protection
- ▶ Disposal of Chemicals
- ▶ Electrical Safety
- ▶ Most Serious Problem
- ▶ Safety Program Planning
- ▶ Safety Information Resources
- ▶ Critique and Closing Comments
- ▶ Additional Questions and Answers

### **ABOUT THE INSTRUCTOR**

**Dr. James A. Kaufman** is President/CEO of The Laboratory Safety Institute (LSI) and former Professor of Chemistry and EHS Director at Curry College. He received his bachelors degree in chemistry from Tufts University and his doctorate in organic chemistry from Worcester Polytechnic Institute (WPI). He is widely regarded as the nation's leading expert on laboratory safety. After two years as a post-doctoral fellow in the WPI Chemical Engineering Department converting garbage into fuel oil, Dr. Kaufman joined the Dow Chemical Company's New England Research Laboratory as a Process Research Chemist. During his four years with Dow, he became increasingly involved in laboratory safety related activities. He authored "Laboratory Safety Guidelines". Originally distributed by Dow, now over two million copies of the widely requested and reprinted brochure are in circulation.

Dr. Kaufman is the founder and President/CEO of The Laboratory Safety Institute – an international, non-profit center for safety in science and science education. LSI's lectures and training programs, AV-lending library, Mini-Grants, Internet discussion list, and publications help both academic and non-academic institutions throughout the world. Over 60,000 scientists and science educators have attended these courses and presentations. LSI is supported, in part, by grants from individuals, foundations, companies and professional societies.

LSI conducts seminars, short courses, audits and inspections for schools, colleges, and companies. They also provide advice on regulatory compliance, safety program development, facilities design, editorial commentary on laboratory texts, and expert witness testimony.

Dr. Kaufman is a former, ten-year member of the American Chemical Society's (ACS) Council Committee on Chemical Safety and is past-chairman of the 2,500-member ACS Division of Chemical Health and Safety. He is the author-narrator of the ACS Audio Course on Laboratory Safety and editor of "Waste Disposal at Academic Institutions" from Lewis Publishers. He recorded and edited the "One-Day Laboratory Safety Audio Seminar" and "Two-Day Lab Safety Video Course." Most recently, he co-authored "Safety Is Elementary: the new standard for safety in the elementary science classroom."

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## **Data Analysis for Improved Productivity in the Analytical Laboratory**

**One-Day Course E11-27, Tuesday, November 15, 2011, 8:30am-5:30pm**

Dr. Zenaida Otero Gephardt, RowanUniversity, Glassboro, NJ

### **COURSE DESCRIPTION**

Statistical techniques are powerful tools that can significantly enhance productivity in the analytical laboratory. Simple statistical analyses can serve to guide experimentation, to identify sources of experimental errors, and to minimize the number of experiments required. The mathematics involved will be presented in a concise manner easily understood by those with a background in science. Basic principles will be discussed in the context of analytical laboratory applications, and a wide range of applications will be discussed. Participants will be able to immediately use the material presented to enhance their effectiveness and productivity in the laboratory.

### WHO SHOULD ATTEND

Analytical chemists at all levels will benefit from this course. Laboratory supervisors and technical personnel involved in data analysis and reporting will also benefit.

### TOPICS

- ▶ Background and Introduction to Data Analysis
- ▶ Precision and Accuracy Calculations and Applications
- ▶ Comparison of Precisions and Applications
- ▶ Comparison of Results and Applications
- ▶ Relationships Between Variables and Applications
- ▶ Analysis of Variances (ANOVA) and Applications
- ▶ Calibration Curves
- ▶ Techniques for Data Comparisons

### ABOUT THE INSTRUCTOR

**Dr. Zenaida Otero Gephardt** is Associate Professor of Chemical Engineering at Rowan University (Glassboro, NJ) and consultant through Otero Keil Associates. Her research focuses on optimization, development and mathematical modeling of chemical processes and laboratory techniques. She has developed statistical models and experimental designs for a wide range of chemical processes including high pressure, supercritical systems and multi-phase systems. Dr. Gephardt has worked with a wide range of system scales ranging from bench scale laboratory systems to large-scale industrial applications. Dr. Gephardt has over 20 years of experience with analysis and optimization applications in the chemical process industry. She teaches on-site courses for industry and provides analysis and experimental design support. Dr. Gephardt holds a Ph.D. in chemical engineering from the University of Delaware and is a registered Professional Engineer in Delaware.

## Interpretation of Mass Spectra with Practical Solutions to Problems

**One-Day Course E11-28, Tuesday, November 15, 2011, 8:30am-5:30pm**

Dr. Birendra N. Pramanik, Merck Research Laboratories, Kenilworth, NJ  
Dr. Mike S. Lee, Milestone Development, Newtown, PA

### COURSE DESCRIPTION

This introductory course covers the theory and practical interpretation of mass spectra of organic compounds and proteins/peptides through the use of practical examples. The principles of interpretation are to be illustrated by various mass spectral data from EI, CI, DCI, FAB, ESI, APCI, MALDI-MS. This course emphasizes problem-solving skills with examples encountered in industrial and academic research, including structural characterization of trace level impurities and degradation products, analysis of natural products, identification of drug metabolites and structural determination of proteins/peptides. This course provides information on methods and technologies, enabling you to address the challenges that come across routinely.

### WHO SHOULD ATTEND

This course is designed for practicing mass spectrometry scientists (new users, experienced professionals, chromatographers, analytical chemists, protein chemists and laboratory managers).

### TOPICS

- ▶ Principles of Interpretation of Mass Spectra
- ▶ Electron Impact
- ▶ Chemical Ionization
- ▶ Desorption Chemical Ionization
- ▶ Fast-atom Bombardment
- ▶ Atmospheric Pressure Ionization (ESI/APCI)
- ▶ Matrix-assisted Laser Desorption Ionization
- ▶ Applications in Problem-solving
- ▶ Examples

### ABOUT THE INSTRUCTORS

**Dr. Birendra N. Pramanik** has been working (for Schering-Plough Research Institute, now Merck Research Laboratories, MRL) in the area of mass spectrometry since 1980. He is currently a Distinguished Fellow at MRL. Dr. Pramanik directs mass spectrometry and NMR efforts in support of the R&D programs. The responsibility of this group is to utilize modern instrumentation (NMR, LC/NMR, HR/MS, EI, GC/MS, LC/MS, LC/MS/MS, FT-MS, UV, IR) to provide structural identification of new chemical entities (small molecules) and therapeutic proteins for the discovery and development of novel pharmaceuticals. He has published over 145 research papers mostly in the area of mass spectrometry, including chapters in books. Dr. Pramanik is a co-editor of a book on "Applied Electrospray Mass Spectrometry" (Marcel Dekker, Inc., New York, 2002). He has been an invited speaker at national and international meetings. He has served as a chairperson for the North Jersey ACS Mass Spectrometry group and as chairman for major sessions of the American Society for Mass Spectrometry meetings. He has received a number of awards, including the American Chemical Society New Jersey Regional Award for Achievements in Mass Spectrometry. He received his Ph.D. in Organic Chemistry under Professor Ajay K. Bose from Stevens Institute of Technology in 1977.

**Dr. Mike S. Lee** is President of Milestone Development Services. He actively participates in the growth of new technologies and their integration into drug development. Dr. Lee has extensive experience with pharmaceutical analysis and drug development. He has pioneered the application of LC/MS in different phases of drug development for research in biomolecules, natural products, drug metabolites, impurities, and degradants. Prior to founding Milestone Development Services, Dr. Lee was with Bristol-Myers Squibb from 1987-1998. As Director of Analytical Research and Development, Dr. Lee was responsible for departments in several research facilities providing MS, NMR, IR, HPLC, CE, and physical chemistry support. He led interdisciplinary teams responsible for rapid analysis of discovery leads and preclinical drug candidates that contributed to the Food and Drug Administration approval of Buspar®, and Serzone®, and the accelerated development and approval of TAXOL®. Dr. Lee has published over 40 research papers and book chapters about the analysis of drugs and related compounds. Dr. Lee's book entitled "LC/MS Applications in Drug Development" was recently published by J. Wiley & Sons. Dr. Lee received his B.S. in Chemistry from the University of Maryland and his M.S. and Ph.D. in Analytical Chemistry from the University of Florida under the direction of Professor Richard A. Yost.

## Troubleshooting Chromatographic Systems

**Two-Day Course E11-29, Wednesday and Thursday, November 16 and 17, 2011, 8:30am-5:30pm**

Dr. Merlin K.L. Bicking, ACCTA, Inc., Woodbury, MN  
Dr. Douglas E. Raynie, South Dakota State University, SD

### COURSE DESCRIPTION

Chromatographic instruments are an integral part of almost every analytical laboratory. While modern instruments are very reliable, chromatographers must still deal with many day-to-day problems (peak shape changes, baseline shifts, retention time problems, etc.) that can arise from the instrument, the sample, or the laboratory. This seminar will provide guidance on identifying the causes of such problems, finding solutions, and preventing future problems. Basic LC and GC components will be discussed, and helpful hints will be provided on how to avoid certain problems and maximize the overall analytical efficiency in the laboratory. Students will learn about general troubleshooting strategies, common symptoms, and common solutions to common symptoms. This seminar provides practical technical information that is not available from any other source.

Students are encouraged to bring examples of problems from their own laboratories for open discussion. This has been one of the most popular courses at EAS over for many years, and regularly receives excellent reviews from participants. Come find out why!

### WHO SHOULD ATTEND

Anyone involved with conducting or managing GC or HPLC analyses.

### TOPICS

- ▶ A General Approach to Troubleshooting
- ▶ Minimizing Errors in Peak Integration
  - How do chromatographic integrators work
  - What integration baseline options are available
  - Understanding the errors and minimizing them
- ▶ GC Troubleshooting
  - Current trends in instrument design
  - Comprehensive troubleshooting strategies for GC
  - Matching symptoms with solutions
- ▶ LC Troubleshooting
  - Current operating issues in HPLC
  - Design-related problems
  - Linking symptoms and solutions with the LC Troubleshooting Matrix
- ▶ Open Discussion
  - Bring your own examples and questions

### ABOUT THE INSTRUCTORS

**Dr. Merlin K. L. Bicking** (Course Director) is President, ACCTA, Inc. He has extensive analytical chemistry experience in academia, contract research, independent testing laboratories, consulting, and technical training. His professional history includes development of two EPA methods, as well as numerous methods in other regulated and non-regulated industries. His publications and presentations cover a wide range of topics, including liquid chromatography theory, derivatization, method optimization, and the use of experimental design strategies in analytical chemistry. He also develops and presents technical training seminars for analytical laboratory staff.

**Dr. Douglas E. Raynie** is a Research Assistant Professor in the Department of Chemistry and Biochemistry at South Dakota State University. Prior to joining SDSU, he was employed for eleven years as a Senior Scientist at Procter and Gamble's Corporate Research Division. He earned his Ph.D. at Brigham Young University under the direction of Dr. Milton L. Lee. His undergraduate degree is from Augustana (South Dakota) College, with majors in chemistry and biology. Analytical separations research in Dr. Raynie's laboratory includes high-resolution chromatography (high-temperature LC and SFC), chromatographic sample preparation (ASE, SFE, SPME, and SPE), chromatography theory, green analytical chemistry, and problem-based learning in analytical chemistry.

## Hands-On FTIR, NIR and Data Analysis – What is the Right Tool to Solve Your Problems

**New Two-Day Course E11-30, Wednesday and Thursday, November 16 and 17, 2011, 8:30am-5:30pm**

Dr. Katherine A. Bakeev, CAMO Software Inc., Woodbridge, NJ  
Dr. Brian C. Smith, Spectros Associates, Shrewsbury, MA

### COURSE DESCRIPTION

This hands-on course will introduce you to FTIR and Near-Infrared (NIR) spectroscopies. For each technique you will learn how the instrument works, its advantages and disadvantages, sample preparation, and applications. You will also see how the data measured with each technique are used and processed. Discover how spectral subtraction and library searching are used in FTIR to help analyze mixtures and identify unknowns. See how FTIR and NIR are used to obtain single analyte calibrations. Discover how chemometric techniques are used to turn NIR spectra into information, such as classifying samples and obtaining quality calibrations from complex mixtures. Through hands-on experiments attendees will learn how to prepare samples, use spectrometers, and analyze spectral data.

### WHO SHOULD ATTEND

Lab technicians, scientists, or managers who use vibrational spectroscopy in their jobs, or are thinking about using it. Anyone who measures vibrational spectra and wants to turn them into information. People who want to know which technique is best for their analysis.

### TOPICS

- ▶ The Basics of FTIR
  - Introduction to infrared spectroscopy – the properties of light, what is an infrared spectrum, and infrared spectroscopy: good and bad points
  - The Advantages of FT-IR – FTIR vs. dispersive spectrometers, signal-to-noise ratio (SNR), the throughput advantage, and the multiplex advantage
  - The Disadvantage of FTIR: Water and CO<sub>2</sub> Peaks
- ▶ How an FT-IR Works
  - Interferometers and interferograms
  - How a spectrum is produced – the Fourier Transform and background and single beam spectra
- ▶ Spectral Processing
  - The laws of spectral processing
  - Spectral Subtraction – theory, optimizing subtraction results, and spotting artifacts
  - Library Searching – background and theory, the search process, and properly interpreting search results
- ▶ Introduction to Quantitative Spectroscopy
  - Derivation of Beer's Law
  - Variables affecting calibrations
  - Calibration and prediction with Beer's Law – introduction to linear regression, measuring calibration accuracy and robustness
  - Standard methods
  - Measuring absorbances properly
  - Avoiding experimental errors – concentration and spectroscopic errors and 15 common experimental pitfalls to avoid
- ▶ Attenuated Total Reflectance (ATR): A Technique for Many Samples
  - Accessory design
  - Variable affecting spectral appearance
  - Applications: polymers, semi-solids: gels, waxes, pastes, etc., liquids, and powders
- ▶ Hands-on FTIR Experiments
- ▶ Near-Infrared (NIR)
  - Basic principles of NIR
  - NIR instrumentation
  - Typical applications of NIR
- ▶ Sampling options for NIR
  - Transmittance
  - Diffuse reflectance
  - Transflectance
  - Probes for *in-situ* analysis
- ▶ NIR Application Examples
  - Quantitative analysis of water
  - Raw material classification library
  - Real-time monitoring
- ▶ Multivariate Data Analysis
  - Overview of chemometrics
  - Samples needed for developing a calibration
- ▶ Spectral Processing
  - Derivatives, scatter correction, and other tools
- ▶ Qualitative Analysis
  - PCA for exploratory analysis and data visualization
  - Classification
- ▶ Quantitative Analysis: Regression Modeling
  - Model validation
  - MLR
  - PLS
- ▶ Compare and Contrast of MIR vs. NIR
- ▶ Hands-On NIR Experiments

### ABOUT THE INSTRUCTORS

**Dr. Katherine A. Bakeev** is currently the Chief Scientist and Product manager for CAMO Software Inc., where she leads the scientific team, drives product management and has responsibilities in supporting the North American market. She has many years of industrial experience in the electronics, chemical and pharmaceutical industries. From 2005-2009, she worked in the Process Analytical Technology and Chemometrics group of GlaxoSmithKline in King of Prussia, PA. Her work experience has included supporting customers in pharmaceutical and chemical industries as a product specialist for Foss NIRSystems and work in process analytical chemistry to enhance process understanding with specialty chemical manufacturer, ISP.

Katherine earned her PhD in Polymer Science and Engineering from the University of Massachusetts in Amherst, and has a Masters in Technology Management from Stevens Institute of Technology, in addition to her BS from Case Western University. She has written articles and given numerous presentations on the use of near-infrared spectroscopy (NIR) and on PAT. She is the editor of the book *Process Analytical Technology: Spectroscopic Tools and Implementation Strategies for the Chemical and Pharmaceutical Industries*, now in its second edition. She is the recipient of the 2007 Craver Award in Applied Vibrational Spectroscopy for her efforts in, and promotion of, near-infrared (NIR) spectroscopy and chemometrics. She has been a member of the Society of Applied Spectroscopy (SAS) since 1993, and is the current national secretary of the organization. She has served on the publication and nominating committees, and serves on the Editorial Board of the journal *Applied Spectroscopy*. She is the past president of the Council for Near Infrared Spectroscopy (CNIRS), a member of the Chairman's Advisory Committee for the International Council for Near-Infrared Spectroscopy (ICNIRS), and a member of the ASTM committees E13 (Molecular Spectroscopy and Separation Science) and E55 (Manufacture of Pharmaceutical Products).

**Dr. Brian C. Smith** is founder and principal of Spectros Associates. He has been a spectroscopist for over 30 years and was employed by Bell Labs and Digilab. He is an experienced trainer; thousands of people have benefited from his instruction as part of Spectros Associates since 1992. Dr. Smith is the author of three popular books on spectroscopy; *Fundamentals of FTIR* and *Infrared Spectral Interpretation* published by CRC Press, and *Quantitative Spectroscopy: Theory and Practice* published by Academic Press. Dr. Smith earned his Ph.D. in Chemistry from Dartmouth College and graduated with highest honors from Rochester Institute of Technology with a B.S. in Chemistry.

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## Essentials of Modern HPLC I and II

### **New Two-Day Course E11-31. Wednesday and Thursday, November 16 and 17, 2011, 8:30am-5:30pm**

Dr. Michael W. Dong, Genentech, Small Molecule Analytical Chemistry, S. San Francisco, CA

#### **COURSE DESCRIPTION**

This is a combination of two one-day courses: Essentials of Modern HPLC I: Fundamentals and Applications, and Essentials of Modern HPLC II: Practice, Operation, Troubleshooting and Method Development. A discount will be offered for the combined course over separately registering for the two one-day courses. See course descriptions for Essentials of Modern HPLC I: Fundamentals and Applications, and Essentials of Modern HPLC II: Practice, Operation, Troubleshooting and Method Development.

#### **WHO SHOULD ATTEND**

Analysts, scientists, researchers, and managers who want to get an updated introduction of modern HPLC practices, instrument operation, maintenance, troubleshooting, method development as well as recent advances including UHPLC. It is recommended that you have a good understanding of general chemistry. Some prior hands-on HPLC experience would be helpful.

#### **TOPICS**

##### **DAY ONE:**

- See Topics listed under Essentials of Modern HPLC I: Fundamentals and Applications

##### **DAY TWO:**

- See Topics listed under Essentials of Modern HPLC II: Practice, Operation, Troubleshooting and Method Development

#### **RECOMMENDED TEXT**

1. M. W. Dong, *Modern HPLC for practicing scientists*, Wiley, June 2006.

#### **ABOUT THE INSTRUCTOR**

See Instructor information under Essentials of Modern HPLC single courses.

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## Essentials of Modern HPLC I: Fundamentals and Applications

### **New One-Day Course E11-32. Wednesday, November 16, 2011, 8:30am-5:30pm**

Dr. Michael W. Dong, Genentech, Small Molecule Analytical Chemistry, S. San Francisco, CA

#### **COURSE DESCRIPTION**

This is a one-day HPLC introductory course at a beginner/intermediate level. This course will provide you with an updated overview and a solid working knowledge of high-performance liquid chromatography (HPLC). The attendees will learn useful theoretical concepts, instrumental fundamentals and operating principles, column basics and selection guide, and key applications in various industries. This is the first part of a two-course series for Modern HPLC introduction. The second part, "Essential of Modern HPLC 2", is a follow-on course that focuses on the practice of HPLC: operation, maintenance, troubleshooting, method development as well as recent developments of HPLC including ultra-high-pressure LC or UHPLC.

### WHO SHOULD ATTEND

Analysts, scientists, researchers, and managers who want to get an updated introduction of modern HPLC fundamentals and its diversified applications. It is recommended that you have a good understanding of general chemistry. Some prior hands-on HPLC experience would be helpful.

### TOPICS

- ▶ Introduction and Basic Concepts
  - History, advantages, limitations, and modes
  - Retention time ( $t_R$ ), retention factor ( $k$ ), separation factor ( $\mu$ ), column efficiency ( $N$ ), column void volume ( $V_M$ ), and resolution ( $R_S$ )
  - Mobile phase factors (organic modifiers, pH, buffers), operating parameters (Flow, Gradient time ( $t_G$ ), column temperature ( $T$ ))
- ▶ HPLC Columns, Trends and Selection Guides
  - Column characteristics and types, packing characteristics (support type, particle size, pore size) and bonding chemistries
  - Trends of shorter and narrower columns packed with small particles, high-purity silica, novel bonding chemistries
  - van Deemter equation
  - Column selections guide
- ▶ HPLC Instrumentation and Operating Principles
  - Solvent delivery system, injector, autosampler, detector (UV/Vis, photodiode array, fluorescence, refractive index, ELSD, ECD, conductivity, and mass spectrometer (MS), and data handling system
  - Instrumental bandwidth
- ▶ Practical Applications of HPLC in Diversified Industries
  - An overview of HPLC applications in diversified industries supported with specific case studies
  - Pharmaceutical: drug discovery to quality control, assay, impurities, and dissolution
  - Food: sugars, fats, organic acids, and additives
  - Environmental: US EPA methods, pesticides, and PAHs
  - Chemical: GPC, plastics, and ion-chromatography
  - Bioseparations and life sciences: proteins, peptides, amino acids, oligonucleotides, nuclei acids, and PCR products

### RECOMMENDED TEXT

1. M. W. Dong, *Modern HPLC for practicing scientists*, Wiley, June 2006.

### ABOUT THE INSTRUCTOR

**Dr. Michael W. Dong** is a Senior Scientist at Genentech, Small Molecule Drug Discovery, South San Francisco, CA. His research interests are in Fast LC, ultra-high-pressure LC, rapid HPLC method development and chiral separations. He was formerly Research Director at Synomics Pharmaceutical Services, Research Fellow/Group Leader at Purdue Pharma, Senior Staff Scientist at Applied Biosystems / Perkin-Elmer, and section-head in Hoechst Celanese. He holds a Ph.D. in Analytical Chemistry from City University of New York and a certificate in Biotechnology (UC Santa Cruz, 2010). He has conducted numerous training courses at national meetings on HPLC, UHPLC, HPLC method development and drug development process. He pioneered Fast LC and has over 80 publications in chromatography, pharm analysis and analytical chemistry. He authored a best-seller in chromatography – “Modern HPLC for Practicing Scientists”, Wiley, 2006 and co-edited Handbook of Pharmaceutical Analysis by HPLC, Elsevier/Academic Press, 2005.

## Anatomy of Modern Reversed- Phase Columns: Understanding Their Role in HPLC

**One-Day Course E11-33, Wednesday, November 16, 2011, 8:30am-5:30pm**

Dr. Brian A. Bidlingmeyer, Agilent Technologies, Inc., Wilmington, DE  
Dr. Richard A. Henry, PennStateUniversity, State College, PA

### COURSE DESCRIPTION

The heart of any HPLC system is the column. Understanding the reversed-phase column contributes greatly to successful separations and rugged HPLC methods. This short course treats the column as the center of the system and focuses on how the column is made, how it contributes to the system and how it is used successfully. Approximately half of the column course will focus on the “nuts and bolts” and will cover topics such as particle size, pore size, the base particle (silica, polymer, hybrid, others), surface chemistries, hardware and geometries. The other half will discuss choosing a column and stationary phase for the task at hand, development of a rugged method, column troubleshooting, and proper column care and use.

### WHO SHOULD ATTEND

This one-day course will benefit analysts, managers, regulators, and researchers, who perform HPLC and evaluate data related to pharmaceutical and other products. It will be particularly useful to those who develop or desire to develop their own HPLC methods. The course was designed for analytical chemists, biochemists and others who have some experience in HPLC. To get the most out of the course, it is highly recommended that you have at least one year of HPLC operating experience.

**TOPICS**

- ▶ Overview of HPLC and role of the column
  - Terminology- Principles of sample retention and resolution (what makes up a column)
  - Types of column backbones
- ▶ How silica is made
- ▶ How silica is bonded
- ▶ How the column is used
- ▶ How to choose the best column and stationary phase for different solutes
- ▶ What changes in UHPLC columns
- ▶ Role of mobile phase, including temperature and viscosity
- ▶ Modes and method development- emphasis on RP
- ▶ Troubleshooting the separation and the column
- ▶ Care and use for long column life
- ▶ General questions from attendees

**ABOUT THE INSTRUCTORS**

**Dr. Brian A. Bidlingmeyer** is employed by Agilent Technologies in Wilmington, DE. He is an accomplished separation scientist who has work experience in the chemical, pharmaceutical and instrumentation industries. He has published 2 books and more than 80 papers. Brian is the Chairman-elect of the Separations Science Subdivision of the American Chemical Society's Analytical Division and is active in the ASTM committee concerning chromatographic practices. He has made significant contributions to the practice and understanding of modern HPLC and has received numerous awards including the Heinrich Emmanuel Merck Prize for contributions to analytical chemistry, the International Ion Chromatography Award for contributions to that area, and an IR 100 Award for a new method for amino acid analysis (Pico Tag Method). He is presently an associate editor of the *Journal of Chromatographic Science*.

**Dr. Richard A. Henry** received his B.S. degree in Chemistry from Juniata College in 1963 and Ph.D. in Analytical Chemistry from The Pennsylvania State University in 1966. After a postdoctoral year in separations at Purdue University with Professor L. B. Rogers, he joined DuPont at the Experimental Station in Wilmington, DE and became one of the first employees of the Analytical Instrument Products Division. Dick worked closely with Dr. Jack Kirkland and others in the development of HPLC columns and packing materials until about 1973. After about 10 years on the west coast with Spectra-Physics, he joined the PennState University chemistry faculty and became Director of Analytical Laboratories where he taught Instrumental Analysis to chemistry majors. He also founded Keystone Scientific, Inc. in 1985 to develop and market HPLC columns and related separation technology. He retired from both PennState University and Keystone Scientific in 2002, and remains active teaching short courses on separation technology and as a consultant. Dick has research interests in separation mechanisms and all applications of the latest HPLC column technology. He has special interest in the rapidly growing fields of UHPLC, chiral HPLC, LC-MS, and multidimensional separation methods. He served two terms as Chairman of the ACS Subdivision on Separations (1998-2002) and has also served on its Executive Committee.

## Practical Headspace Gas Chromatography

**One-Day Course E11-34, Wednesday, November 16, 2011, 8:30am-5:30pm**

Dr. Mary Ellen P. McNally, DuPont, Wilmington, DE  
Dr. Thomas A. Brettell, Cedar Crest College, Allentown, PA

**COURSE DESCRIPTION**

Headspace sampling is an established technique for volatile sample introduction in chromatography. When complicated sample matrices make sample preparation difficult, the gas headspace above the sample is a valuable source of information. Accurately measuring this gas phase can be challenging. Specifically, the challenges are establishing a representative sample, devising an accurate calibration for the matrix of interest and replicate analyses from a static system. These topics as well as discussions on theory, appropriate apparatus and instrumentation, and applications from the pharmaceutical industry (specifically addressing the new USP467 Guidelines), forensic science, manufacturing, environmental, and food and flavor industry will be presented in this course.

**WHO SHOULD ATTEND**

This one-day course will benefit method development scientists, R&D analysts, R&D formulators, QC analysts, regulatory affairs associates, R&D, RA and QA/QC managers for both bulk drug and finished dosage form developers and manufacturers.

**TOPICS**

- ▶ Introduction
  - Introduction and background of speakers
  - Logistics
  - Course outline/scope of course
  - Course materials
- ▶ Theory: Basic Principles of Headspace GC
  - Partition ratio
  - Phase ratio
  - Physical chemical aspects
- ▶ Multiple headspace extraction
  - Static headspace
  - Passive headspace
    - SPME
  - Dynamic headspace (Purge and Trap)
  - Headspace single drop microextraction Techniques
- ▶ Instrumentation
  - Gas tight injection
  - Balanced-pressure system

- Pressure-loop system
- Sample preparation
- Sample vials
- ▶ Quantitation
- ▶ System Optimization/Troubleshooting
  - Transfer line
  - Interfaces
- ▶ Applications
  - Pharmaceutical applications
  - <USP467>
  - European pharmacopoeia tests
  - Forensic applications
    - Blood alcohol determination
  - Environmental applications
  - Manufacturing/industrial applications
  - Food and flavor applications
- ▶ Wrap Up/Reflections/Discussion

### ABOUT THE INSTRUCTORS

**Dr. Mary Ellen P. McNally** (Course Director) is a Technical Fellow at the Stine Haskell Research Center for the Crop Protection Products business unit of E.I. du Pont de Nemours & Co., Inc. in Newark, DE. Her main research areas are in the fields of separations, sample preparation and sensors. Most of her work has been focused in the environmental area, both in environmental fate of agricultural products, ultra-trace level analysis and detection as well as analysis associated with manufacturing and process development. Her Ph.D. thesis was in the area of Headspace analysis of priority pollutants. Dr. McNally received the American Microchemical Society Steyermark Award for her work conducted in the field of microanalysis, the Chromatography Forum of Delaware Valley Award for contributions to theory, instrumentation and applications to the field of chromatography and service to the organization. Mary Ellen has been recognized for her contributions to the field of supercritical fluids by the Midwest Supercritical Fluid Chromatography Discussion and the Tri-State Analytical Supercritical Fluid Discussion Groups. Dr. McNally is a member the editorial advisory board for *LCGC* magazine and a former member of the Instrumentation Panel and the Advisory Board for the journal of Analytical Chemistry and the editorial board of *Talanta*. Within DuPont, Dr. McNally has received DuPont's highest award for contributions to trace level analysis as well as the DuPont Scientific Leadership Award. This award afforded her the opportunity to work at the ImperialCollege in London in capillary electrochromatography as well as LC and CE on a microchip and at the Molecular Engineering Cooperative Research Center of CSIRO in Sydney Australia working in the area of biosensors.

**Dr. Thomas A. Brettell** retired in 2007 as the Director of the New Jersey State Police Office of Forensic Sciences and is presently an Assistant Professor in the Chemical and Physical Sciences Department at CedarCrestCollege. Dr. Brettell's main research areas are in chromatography and medico-legal aspects of alcohol. His Ph.D. thesis was in the area of Headspace Gas Chromatographic analysis of fire debris accelerants. He has taught advanced separation courses and has taught in the gas chromatography course sponsored by the Chromatography Forum of the DelawareValley. In 1993, he received a commendation from the NJSP Superintendent for his work on a narcotics investigation. Dr. Brettell is the past Chair of the Criminalistics Section of the American Academy of Forensic Sciences and the past President of the Chromatography Forum of the DelawareValley. Tom was presented the Chromatography Forum of the Delaware Valley Award in 1997 for service to the Forum and accomplishments in the field of separation science, and also served on the Advisory Board of the Journal of Analytical Chemistry from 1996 to 1998. In 2004, Dr. Brettell was appointed to the Governor's Advisory Council Against Sexual Violence and served until 2006. He presently serves on the National Safety Council's Committee on Alcohol and Other Drugs. Dr. Brettell is a certified Diplomat of the American Board of Criminalistics and a Fellow in the AmericanAcademy of Forensic Sciences.

## Analytical Metrology

**New One-Day Course E11-35, Wednesday, November 16, 2011, 8:30am-5:30pm**

Dr. Jerry D. Messman, Stranaska Scientific LLC, Fort Collins, CO

### COURSE DESCRIPTION

Metrological practices with respect to chemical analysis are becoming more rigorous because of formalized measurement assurance programs and the evolving emphasis on international standardization and laboratory accreditation. Analytical metrology broadly encompasses many measurement operations including analytical instrument qualification, analytical methods testing (chemical metrology or metrology in chemistry), and physical properties characterization. This course provides a basic introduction to many facets of the overall analytical measurement process including calibration, reference material standardization, traceability, estimation and reporting of measurement uncertainty, and how they together can impact the quality and reliability of measurement results and the confidence in any consequential actions or decisions. Much of the course material is gleaned from authoritative international references. Instruction is provided from a broad perspective to make it relevant to a wide range of analytical laboratories including those in the biotech, chemical, clinical, environmental, food and beverage, forensic, industrial hygiene, petrochemical, and pharmaceutical industries.

### WHO SHOULD ATTEND

This course is intended for laboratory analysts, technicians, supervisors and managers who have metrological responsibilities for ISO 17025 accreditation, analytical methods testing, quality assurance and internal quality audits. It is also beneficial to metrologists, calibration specialists, and instrument service technicians who must demonstrate technical competence in analytical instrument qualification.

**TOPICS**

- ▶ Metrological Definitions, Terms and Concepts
- ▶ Key Government Agencies and International Organizations
- ▶ Measurement Scales and Units
- ▶ Calibration Hierarchy
- ▶ Reference Material Standards
- ▶ Metrological Traceability
- ▶ Measurement Uncertainty
- ▶ Analytical Methods Testing (Chemical Analysis)
- ▶ Analytical Instrument Qualification: UV/VIS/NIR, IR/Raman, Fluorescence, HPLC

**ABOUT THE INSTRUCTOR**

**Dr. Jerry D. Messman** holds a Ph.D. degree in analytical chemistry from the University of Maryland (College Park, MDUSA). Jerry has been involved in various spectrometric aspects of analytical chemistry and metrology throughout his entire professional career beginning 30 years ago with the National Bureau of Standards (NBS). During his tenure at the National Institute of Standards and Technology (NIST) from 1988 to 1992, Jerry was responsible for rejuvenation of the high-accuracy spectrophotometric standards program in the Chemical Sciences and Technology Laboratory. During that time, he directed all NIST technical activities involving the production, certification, and recertification of UV/VIS spectrophotometric Standard Reference Material (SRM) artifacts. For the past 17 years, Jerry has served as Managing Director and Senior Scientist of Stranaska Scientific LLC, an analytical research and development company dedicated to the scientific and educational advancement of analytical metrology worldwide. Jerry is an elected member of CITAC, an acronym for the Cooperation on International Traceability in Analytical Chemistry.

**High-Throughput Drug Analysis by LC/MS**

***New One-Day Course E11-36, Wednesday, November 16, 2011, 8:30am-5:30pm***

Dr. Perry G. Wang, United States Food and Drug Administration, College Park, MD

**COURSE DESCRIPTION**

The introduction of combinatorial chemistry technology has significantly increased the amount of compounds generated in pharmaceutical industry. Conventional analytical approaches simply cannot keep up. These circumstances have caused drug discovery and development to take on the shape of a bottleneck, like traffic through a toll booth. In order to break the bottleneck, a corresponding revolutionary improvement to the conventional methodology must happen.

High-throughput drug analysis is a new topic for drug discovery and development in the pharmaceutical industry. This one-day short course will mainly focus on the most recent significant advances of high-throughput sample preparation and drug analyses by LC/MS.

**WHO SHOULD ATTEND**

This one-day course will benefit the scientists ranging from college students to professionals in the fields of pharmaceutical industry and biotechnology.

**TOPICS**

- ▶ Overview
  - Introduction of high-throughput concept to pharmaceutical industry
  - Why do we need high-throughput analysis
  - The requirements for high-throughput analysis
  - Why do we use LC/MS or LC/MS/MS
- ▶ How to Develop a High-Throughput LC/MS Method
  - The relationship of pKa and pH
  - MS analyzer selection and MS parameters optimization
  - HPLC,  $\mu$ HPLC and UHPLC
  - Solvent selection
  - Introduction of nanoelectrospray technology
  - Introduction of HPLC-Chip/MS system
  - Introduction of multiplexing systems
- ▶ High-Throughput Sample Preparation
  - Protein precipitation
  - Liquid-liquid extraction
  - Solid phase extraction
  - Immobilized liquid extraction
  - Introduction to solid phase micro extraction
  - Disposable pipette extraction - DPX
- ▶ Special Topics
  - Monolithic chromatography for high-throughput analysis
  - Hydrophilic interaction liquid chromatography (HILIC) for biological samples
  - Ion suppression of biological samples
  - How to deal with urine samples

**ABOUT THE INSTRUCTOR**

**Dr. Perry G. Wang** is a research chemist in the Office of Regulatory Science, Center for Food Safety and Applied Nutrition, US Food and Drug Administration (US FDA). His interests include analytical method development and validation for drugs and constituents of foods and cosmetic products using advanced instrumentation. His expertise focuses on high throughput drug analysis by LC/MS/MS for the pharmaceutical industry.

Recently, he has published three books: his first book entitled "High-Throughput Analysis in the Pharmaceutical Industry" was published by CRC Press in October 2008; his second book entitled "Monolithic Chromatography and Its Modern Applications" was published by ILM Publications in September 2010; and his third book entitled "Hydrophilic Interaction Liquid Chromatography (HILIC) and Advanced Applications" was published in March 2011 by CRC Press. He is currently editing another book entitled "Identification and Analysis of Counterfeit and Substandard Pharmaceuticals" with ILM Publications, which is scheduled for publication in October 2011.

He has prepared, organized and presided over symposia for the Pittsburg Conference (PittCon) since 2006. He has been an invited speaker since 2004 at international conferences including the PittCon; Federation of Analytical Chemistry and Spectroscopy Societies (FACSS); Beijing Conference and Exhibition on Instrumental Analysis (BCEIA) and International Symposium on Chemical Biology and Combinatorial Chemistry (ICCBCC). He has been invited to teach short courses for the PittCon, the American Chemistry Society (ACS) Annual Meetings, and Eastern Analytical Symposium (EAS). His current research focuses on developing analytical methods for constituents of cosmetics and dietary supplements.

Dr. Wang received his B.S. degree in Chemistry from Shandong University. He earned his M.S. and Ph.D. degrees in Environmental Engineering from Oregon State University, in Corvallis, Oregon, USA

## Practical Enantiomeric Separations

**New One-Day Course E11-37, Wednesday, November 16, 2011, 8:30am-5:30pm**

Dr. Daniel W. Armstrong, University of Texas, Arlington, TX

### COURSE DESCRIPTION

Chirality is an inherent property of all living things. Hence, enantiomers that have the same physical and chemical properties (except for the rotation of plane polarized light) in an isotropic environment tend to have different biological properties. Consequently, the analysis, isolation, use, and production of enantiomers is of fundamental importance in many areas of science and technology. This course will provide a basic introduction and background to chirality and a survey of the methodologies used in enantiomeric separations and analysis. There will be an emphasis on separations of interest to pharmaceutical and environmental chemists. The newest chiral selectors will be covered, as well as supercritical fluid (SFC) separations and chiroptical detectors.

### WHO SHOULD ATTEND

This one-day course will benefit pharmaceutical scientists, organic chemists, analytical chemists, biochemists, food scientists, environmental scientists, regulators, and QC managers. It is assumed that everyone attending this course has a good basic knowledge of organic chemistry and chromatography.

### TOPICS

- ▶ History and Nomenclature
- ▶ HPLC Chiral Stationary Phases
- ▶ Chiral SFC
- ▶ Chiroptical Detectors
- ▶ Chiral Gas Chromatography

### ABOUT THE INSTRUCTOR

**Dr. Daniel W. Armstrong** is the Robert A. Welch Professor of Chemistry at the University of Texas at Arlington, TX. He received his B.S. (1972) from Washington and Lee University and his M.S. (1974) and Ph.D. degrees (1977) from Texas A&M University. He has over 500 publications including 22 book chapters, 1 book (Use of Ordered Media in Chemical Separations) and 12 patents. He has given over 460 invited seminars and colloquia worldwide. He is considered the "Father" of pseudophase (micelle and cyclodextrin-based) separations. He elucidated the first chiral recognition mechanism for cyclodextrins. He also first developed macrocyclic antibiotics as chiral selectors.

He is one of the world's leading authorities on the theory, mechanism, and use of enantioselective molecular interactions. Over 30 different LC and GC columns originally developed in his laboratories have been commercialized and/or copied worldwide. His work and columns were in part responsible for the chromatography and electrophoresis-lead revolution in chiral separations over the last two decades. This work provided the impetus for the FDA's regulatory changes regarding chiral drug development in 1992. More recently, he has developed rapid, high efficiency, microfluidic methods for analyzing microorganisms and colloidal particles. Dr. Armstrong also developed the most comprehensive solvation and characterization models for room temperature ionic liquids (RTILs) and pioneered their use in analytical chemistry. He has received over 20 awards for research and teaching.

## Residual Solvents Testing: Strategies to Meet the USP<467> Requirements

**New One-Day Course E11-38, Wednesday, November 16, 2011, 8:30am-5:30pm**

Mr. Gregory Martin, Complectors Consulting, Pottstown, PA

### **COURSE DESCRIPTION**

This course is designed to provide participants with an understanding of the global requirements for residual solvents testing and practical strategies to meet the requirements, using resource-sparing approaches when appropriate. It will include a review of the compendial analytical methods, and discussion on use of alternative methods. There will be ample opportunity to discuss questions and challenges from the participants.

Upon completion of this course the learner should be able to:

1. Understand the requirements for residual solvents in the US, EU and Japan
2. Implement a testing program to assure compliance with the requirements, using compendial or alternative methods
3. Utilize strategies to minimize the testing and resources required to meet the requirements

### **WHO SHOULD ATTEND**

This one-day course will benefit Chemists (Research, Quality Control, CRO) involved with residual solvents testing and their managers, and regulatory affairs/CMC personnel responsible for documenting compliance with residual solvents requirements.

### **TOPICS**

- ▶ Regulatory Landscape
  - ICH, USP, EP and JP
  - Recent guidance from FDA
- ▶ Practical Implementation of the Requirements
  - Classification of solvents: Class 1, 2 and 3
  - Options for compliance
  - Decision tree
- ▶ Analytical Methods
  - Compendial procedures
  - Alternative methods
- ▶ Risk Based Strategies to Minimize Testing and Resources
- ▶ Common Issues and Practical Solutions
  - Managing suppliers and CROs
- ▶ Review of Course Contents
- ▶ Interactive Session
  - Questions and answers
  - Situations encountered by the audience

### **ABOUT THE INSTRUCTOR**

**Mr. Gregory Martin** is President of Complectors Consulting, which provides consulting services and technical training related to pharmaceutical analysis, regulatory and compendial issues and improving lab efficiency. He has 30 years of experience in the pharmaceutical industry, including 25 years at a major PhRMA company where he was Director of Pharmaceutical Analytical Chemistry in an R&D laboratory supporting new product development. He has developed and presented courses on Residual Solvents for several organizations, including USP and University of Wisconsin Extension School, and worked with several firms to develop practical, resource-sparing programs to assure compliance with residual solvents requirements. He has had significant impact on USP <467> in his role as Vice Chair of USP General Chapters (Physical Analysis) Expert Committee.

In addition, Mr. Martin has significant interest in dissolution testing, analytical method lifecycle (design, development, validation and transfer), control of impurities and degradation products, analytical instrument qualification and strategies for addressing cGMP compliance in the laboratory.

## Fundamentals of Gas Chromatography for New Analysts and Non-Chemists

**New One-Day Course E11-39, Wednesday, November 16, 2011, 8:30am-5:30pm**

Dr. Harold McNair, Virginia Tech, Blacksburg, VA  
Dr. Nicholas Snow, Seton Hall University, South Orange, NJ

### **COURSE DESCRIPTION**

This is a basic course on the fundamentals of operating, maintaining and troubleshooting gas chromatographs. It is intended for new users who may or may not be experts in chemistry. Emphasis will be placed on setting up, operating and the basics of maintaining gas chromatographs. A workshop on troubleshooting and hands-on experience with installing capillary columns and working with the various fittings and consumables will be included. No experience with gas chromatography, but a desire to learn, is needed for this course.

### WHO SHOULD ATTEND

This one-day course will benefit the following:

- New users of gas chromatography
- Analysts with degrees other than in chemistry
- Analysts with chemistry degrees but little background in gas chromatography
- Analysts that would like to learn and practice hands-on techniques in gas chromatography

### TOPICS

- ▶ The Fundamentals of how GC is used to Perform Separations and Analysis
- ▶ The Basics of Troubleshooting Gas Chromatographs
- ▶ Questions to ask the Service Engineer
- ▶ How to Prevent Problems
- ▶ Hands-On: How to Handle and Install Capillary Columns
- ▶ Hands-On: How to Handle and Install Graphite Ferrules
- ▶ Hands-On: How to Maintain and Keep your GC Clean
- ▶ Workshop: Troubleshooting from Instrument Symptoms

### ABOUT THE INSTRUCTORS

**Dr. Harold McNair** is professor emeritus of Analytical Chemistry at Virginia Tech, Blacksburg, Virginia. His research interests are the isolation, concentration and characterization of trace organic molecules by GC, LC and GC/MS. Analytes of interest include pesticides in water, soil and food; biogenic amines in fish; PNA's and PCB's in water and soil; and bomb residues in all types of matrices. He has published over 156 technical papers, 8 books and 14 chapters on chromatography. He has directed the thesis work of 63 graduate students, supervised over 50 post-doctoral fellows and 80 undergraduates.

Prof. McNair has taught a variety of graduate and undergraduate classes at Virginia Tech for 34 years. He also introduced the ACS short courses in GC, LC and GC/MS at Virginia Tech and has taught over 80 of them in the past 35 years. He has actively consulted for many industries as well as EPA, FDA, FBI and TSA.

He has received a variety of national and international awards for both teaching and research, among them: Tswett Medal from the Russian Academy of Science, Keene Dimick Award and Dal Nogare Awards (Pittsburgh Conference), EAS Awards in both Chromatography and Analytical Chemistry, the Colacro Medal from South America and the ACS J.C. Giddings award in Teaching. Most recently, 2009, he received the Lifetime Achievement Award for Chromatography from LC/GC magazine.

**Dr. Nicholas Snow** is Professor and Chair of the Department of Chemistry and Biochemistry and Director of the Center for Academic Industry Partnership at Seton Hall University, South Orange, NJ. His entire education from first grade through PhD was in the Commonwealth of Virginia. He holds a BS in Chemistry from the University of Virginia and a PhD from Virginia Tech where he worked under the Direction of Prof. Harold McNair on computer simulations of gas chromatographic retention. He performed postdoctoral work in forensic toxicology at the University of Virginia prior to his arrival at Seton Hall in 1994. Over the past 15 years he has published 45 research articles and book chapters on many aspects of separation science, most notably gas chromatography and sample preparation. His research group has active projects in fundamental gas chromatography, LCxGC, GCxGC, SPME, GC-MS and ion mobility spectrometry with application areas including drugs, solvents, flavors and fragrances. He is especially interested in broadening the classes of compounds amenable to GC and GC-MS analysis. He is a member of the Governing Board of the Eastern Analytical Symposium and was its President in 2001. He chaired Seton Hall's university-wide Middle States re-accreditation in 2004 and he has been recognized twice by Seton Hall's Board of Regents for outstanding teaching and service to students.

## **Essentials of Modern HPLC II:**

### **Practice, Operation, Troubleshooting and Method Development**

**New One-Day Course E11-40, Thursday, November 17, 2011, 8:30am-5:30pm**

Dr. Michael W. Dong, Genentech, Small Molecule Analytical Chemistry, S. San Francisco, CA

### COURSE DESCRIPTION

This is a one-day HPLC introductory course at a beginner/intermediate level. This course will introduce you to best practices of high-performance liquid chromatography (HPLC) as well as tricks-of-the-trade for successful HPLC operation. The attendees will learn step-by-step guide to operating HPLC modules, maintenance procedures, troubleshooting strategies, traditional and accelerated method development processes as well as recent advances of this pervasive analytical technique including a section on ultra-high-pressure LC. This is the second part of a two-course series to Modern HPLC introduction. "Essentials of Modern HPLC I" introduces HPLC fundamental concepts, columns, instrumentations and applications, is a prerequisite for "Essentials of Modern HPLC II".

**WHO SHOULD ATTEND**

Analysts, scientists, researchers, and managers who want to get an updated introduction of modern HPLC practices, instrument operation, maintenance, troubleshooting, method development as well as recent advances including UHPLC. It is recommended that you have a good understanding of general chemistry. Some prior hands-on HPLC experience would be helpful. "Essentials of Modern HPLC I" is a prerequisite to "Essentials of HPLC II" for newer users.

**TOPICS**

- ▶ HPLC Operation
  - Safety and environmental concerns
  - Mobile phase preparation
  - Best practice in HPLC operation
  - Guidelines for increasing HPLC precision and for trace analysis
  - Qualitative and quantitative strategies
- ▶ HPLC Maintenance and Troubleshooting
  - Common HPLC maintenance procedures
  - Problem diagnosis and troubleshooting guide
  - Diagnosing and solving problems (pressure, baseline, peak, data performance)
  - Case studies
- ▶ HPLC Method Development and Validation
  - Tradition strategy for method development
  - 3-pronged template approach for efficient method development
  - Method prequalification and validation
  - Modern trends – software tools and automated systems
- ▶ Novel Approaches and Ultra-High-Pressure LC
  - High-purity silica, novel bonding chemistries, and hybrids
  - HILIC, monolith, sub-3 $\mu\text{m}$  and sub-2  $\mu\text{m}$  packing, fused core particles
  - Ultra high-pressure LC – performance, perspectives and potential issues

**RECOMMENDED TEXT**

1. M. W. Dong, *Modern HPLC for practicing scientists*, Wiley, June 2006.

**ABOUT THE INSTRUCTOR**

**Dr. Michael W. Dong** is a Senior Scientist at Genentech, Small Molecule Drug Discovery, South San Francisco, CA. His research interests are in Fast LC, ultra-high-pressure LC, rapid HPLC method development and chiral separations. He was formerly Research Director at Synomics Pharmaceutical Services, Research Fellow/Group Leader at Purdue Pharma, Senior Staff Scientist at Applied Biosystems / Perkin-Elmer, and section-head in Hoechst Celanese. He holds a Ph.D. in Analytical Chemistry from City University of New York and a certificate in Biotechnology (UC Santa Cruz, 2010). He has conducted numerous training courses at national meetings on HPLC, UHPLC, HPLC method development and drug development process. He pioneered Fast LC and has over 80 publications in chromatography, pharm analysis and analytical chemistry. He authored a best-seller in chromatography – "Modern HPLC for Practicing Scientists", Wiley, 2006 and co-edited Handbook of Pharmaceutical Analysis by HPLC, Elsevier/Academic Press, 2005.

**Quantitative Analysis for Managers, Data Reviewers and Auditors**

**New One-Day Course E11-41, Thursday, November 17, 2011, 8:30am-5:30pm**

Dr. Nicholas Snow, Seton Hall University, South Orange, NJ  
Dr. Gregory Slack, Clarkson University, Potsdam, NY

**COURSE DESCRIPTION**

Analytical chemistry managers today face the unique challenge of supervising laboratories that may at their location or may be spread across the world. The data and methods they must review and approve may be collected at sites far removed from their own location. Data reviewers and auditors face similar challenges. This course will focus on techniques for reviewing data and methods, with an eye toward spotting potential trouble that could lead to investigations and out of specification results.

**WHO SHOULD ATTEND**

This one-day course will benefit the following:

- Managers who must quickly review and approve assay and method development data and results
- Data reviewers who evaluate quantitative results from analytical laboratories
- Auditors who review and comment on quantitative laboratory procedures
- Analysts who desire further grounding in the fundamentals of good quantitative analysis

Some experience in chromatography and/or quantitative analysis is recommended

**TOPICS**

- ▶ How to Spot Potential Trouble in Proposed New Methods
- ▶ How to Troubleshoot and Optimize Methods that are not always Performing to Requirements
- ▶ The Benefits and Pitfalls of Internal Standard, Standard Addition and External Standard Calibration
- ▶ How to use Propagation of Errors to Evaluate Procedures
- ▶ How to Choose the Right Combination of Glassware, Sample Preparation and Instrumental Analysis
- ▶ How to Address Challenges in New Method Validation and Transfer

**ABOUT THE INSTRUCTORS**

**Dr. Nicholas Snow** is Professor and Chair of the Department of Chemistry and Biochemistry and Director of the Center for Academic Industry Partnership at SetonHallUniversity, South Orange, NJ. His entire education from first grade through PhD was in the Commonwealth of Virginia. He holds a BS in Chemistry from the University of Virginia and a PhD from Virginia Tech where he worked under the Direction of Prof. Harold McNair on computer simulations of gas chromatographic retention. He performed postdoctoral work in forensic toxicology at the University of Virginia prior to his arrival at Seton Hall in 1994. Over the past 15 years he has published 45 research articles and book chapters on many aspects of separation science, most notably gas chromatography and sample preparation. His research group has active projects in fundamental gas chromatography, LCxGC, GCxGC, SPME, GC-MS and ion mobility spectrometry with application areas including drugs, solvents, flavors and fragrances. He is especially interested in broadening the classes of compounds amenable to GC and GC-MS analysis. He is a member of the Governing Board of the Eastern Analytical Symposium and was its President in 2001. He chaired Seton Hall's university-wide Middle States re-accreditation in 2004 and he has been recognized twice by Seton Hall's Board of Regents for outstanding teaching and service to students.

**Dr. Gregory Slack** is the Director of Research and Technology Transfer at ClarksonUniversity. As director of the Division of Research and Technology Transfer, he oversees the conduct and promotion of all research activities at the University. Dr. Slack received his Ph.D. in Analytical Chemistry from Virginia Polytechnic Institute and StateUniversity, Blacksburg, Virginia. He earned a Bachelor of Arts degree from the State University of New York at Potsdam. He has over 13 years of experience in the pharmaceutical industry serving increasingly responsible research and manufacturing roles at Dupont, Bristol-Myers Squibb and most recently at Wyeth Pharmaceuticals. Slack has also had academic experience, serving as adjunct research assistant professor of Chemistry at Clarkson, adjunct professor at SUNY Plattsburgh and instructor of Analytical Chemistry at the University of Massachusetts, Lowell, Continuing Education. He has authored or co-authored numerous publications and presented at professionalconferences.

## Practical Solutions to Characterization of Protein Therapeutics Using Mass Spectrometry

***One-Day Course E11-42, Thursday, November 17, 2011, 8:30am-5:30pm***

Dr. Guodong Chen, Bristol-Myers Squibb, Princeton, NJ

Dr. Li Tao, Bristol-Myers Squibb, Hopewell, NJ

**COURSE DESCRIPTION**

This introductory course covers the theory and practical implementation of mass spectrometry (MS) techniques for characterization of protein therapeutics in the laboratory. It emphasizes problem-solving skills with examples encountered in biopharmaceutical industries, including characterization of chemical modifications and post-translational modifications of protein therapeutics. The interpretation of proteins/peptides mass spectra will be illustrated with practical examples. This course will focus on electrospray ionization (ESI) and matrix-assisted laser desorption / ionization (MALDI) techniques in protein analysis, and will survey the various mass analyzer options for characterization of protein therapeutics. A thorough coverage of approaches toward method development for both qualitative and quantitative analysis of protein therapeutics will provide a good starting point for understanding practical issues facing implementation of MS techniques in the laboratory.

**WHO SHOULD ATTEND**

This course is designed for practicing analytical scientists (new users, chromatographers, analytical chemists, protein chemists, and laboratory managers) performing/supporting recombinant protein characterization/analysis, in-process testing, quality control, quality assurance, research and development, and manufacturing.

**TOPICS**

- ▶ Introductions to Mass Spectrometry (MS)
  - Ionization
  - Electrosprayionization (ESI)
  - Matrix-assisted laser desorption / ionization (MALDI)
  - Mass spectra of proteins / peptides
  - Peptide fragmentation
- ▶ Commonly Used Mass Analyzers
  - Quadrupoles
  - Ion trap
  - Ion cycotronresonance (ICR)
  - Time-of-Flight
  - Orbitrap

- Tandem MS (MS/MS)
- Activation methods for proteins/peptides
- ▶ MS Method Development
  - Issues, peptide mass fingerprinting
  - LC/MS
  - MALDI-MS
- ▶ Characterization of Protein Therapeutics
  - Oxidation
  - Deamidation
  - Glycosylation
  - Chemical modification
  - Pegylation / conjugation
- ▶ Quantitative Analysis of Protein Therapeutics
  - Quantification of post-translational modifications
  - *In vivo* quantitation
- ▶ Case Studies

### ABOUT THE INSTRUCTORS

**Dr. Guodong Chen** (Course Director) has extensive pharmaceutical research experience in major pharmaceutical companies, including Eli Lilly and Co., Schering-Plough (now Merck) and Bristol-Myers Squibb. He is currently heading a mass spectrometry group at Bristol-Myers Squibb's Princeton site, providing mass spectrometric/analytical support to drug discovery and development programs in small molecule pharmaceuticals and biologics. He is the author and/or co-author of over 50 research publications in peer-reviewed journals and book chapters, covering the broad area of mass spectrometry and analytical sciences. He has over 65 presentations at conferences and academic institutes. He also organized/chaired scientific sessions at various forums, including major sessions on small molecule pharmaceuticals and biologics at EAS, Pittcon, ASMS conference and ACS conference. Dr. Chen was the Chairperson of the North Jersey Section of ACS Mass Spectrometry Discussion Group (2004) and in 2006, he received Early Career Award in Mass Spectrometry. He was an invited Analytical Chemistry Program Chair for ACS MARM Conference (2005) and elected President of Chinese American Chemical Society-Tri State (2007). He serves as founding coordinator for ASMS Protein Therapeutics Interest Group (2009-2011). Dr. Chen received his Ph.D. in Analytical Chemistry from Purdue University under the direction of Professor R. Graham Cooks.

**Dr. Li Tao** is a Group Leader in the Department of Biologics Product and Process Development, at Bristol-Myers Squibb Co. His group is responsible for biophysical characterization of protein therapeutics using mass spectrometry, chromatography, and spectroscopic techniques. Dr. Tao's group works on protein therapeutics from late stage discovery, through in-process testing, comparability, and stability studies during development, to eventual post-market commitment studies. Dr. Tao received a B.S. in Chemistry in 1986, a M.S. in Physical Chemistry in 1989, both from the University of Science and Technology of China. Dr. Tao received his Ph.D. in Analytical Chemistry from the University of Florida under the direction of Dr. Robert T. Kennedy in 1998. During his graduate studies, he developed several fast immunoassay systems based on capillary electrophoresis and laser-induced fluorescence detection. He also performed on-line monitoring of insulin release from a single islet using the system he developed. Since joining BMS in 1998, Dr. Tao has been with both drug discovery and drug development organizations, working on recombinant therapeutic targets and recombinant protein therapeutics. His work has been focusing on characterization and analysis of recombinant proteins using mass spectrometry. Dr. Tao also has hands-on experience in microbial fermentation and protein purification for recombinant protein production in an industry setting. Dr. Tao is an author/co-author for 15 peer-reviewed publications or book chapters.

## Practical Introduction to Raman Spectroscopy

**One-Day Course E11-43, Thursday, November 17, 2011, 8:30am-5:30pm**

Dr. Frederick H. Long, President Spectroscopic Solutions, LLC., Randolph, NJ

### COURSE DESCRIPTION

Spectroscopic methods such as Raman Spectroscopy have become important tools for at line and on line analysis in a variety of industries and will become increasing more common in the pharmaceutical industry in the near future. This class will provide an overview of Raman spectroscopy. The class will cover basic instrumentation issues and an introduction to the chemometrics and multivariate analysis required to make these instruments useful in a research, QC, or manufacturing setting. Numerous examples and case studies will be presented including raw material identification, process monitoring, and quantitative chemical imaging of coatings. Relevant FDA and USP guidance for instrument qualification and method validation will also be discussed.

### WHO SHOULD ATTEND

Chemists, Engineers, and Quality professionals who need to learn the basics of Raman spectroscopy. This class is ideally suited for someone who may purchase a Raman spectrometer in the near future.

### TOPICS

- ▶ Introduction
- ▶ Primer on NIR and Raman Spectroscopy
- ▶ Instrumentation Issues
- ▶ Chemometrics and Multivariate Analysis
- ▶ Example Applications and Case Studies
- ▶ Method Validation
- ▶ FDA Guidance and USP Requirements
- ▶ Demonstration of Chemometrics Software
- ▶ Summary and Wrap-up

**ABOUT THE INSTRUCTOR**

**Dr. Frederick H. Long** established Spectroscopic Solutions in the summer of 2001. Spectroscopic Solutions provides consulting and training in the areas of process analytical technology, spectroscopy, and statistics for regulated and non-regulated industries. His firm has done work for numerous international pharmaceutical, consumer health-care companies, and scientific instrumentation suppliers. Recently Dr. Long has taught classes at EAS and PITTCO on Near IR spectroscopy, process analytical technology, and quality by design. He received his S.B. and S.M. in Physics from the Massachusetts Institute of Technology and a Ph.D. in Chemical Physics from Columbia University.

## **Dissolution: A Rational Approach to Developing and Validating Methods for a Variety of Purposes**

**One-Day Course E11-44, Thursday, November 17, 2011, 8:30am-5:30pm**

Mr. Gregory Martin, Complectors Consulting, Pottstown, PA

**COURSE DESCRIPTION**

Dissolution testing plays multiple roles for drug products, throughout the product lifecycle from early development to mature marketed product, including generics. This course provides an in-depth and interactive presentation on developing and troubleshooting dissolution methods for a variety of applications, including early development, biorelevant dissolution, *in-vivo/in-vitro* comparisons and marketed products. Real world examples of methods, issues, (sometimes unexpected) testing results and interpretation of data will be used, and there will be ample opportunity for discussion by participants both throughout the course and at the end.

**WHO SHOULD ATTEND**

Scientists who develop or apply dissolution methods (e.g. stability, quality control) and those who need to understand dissolution testing and its implications for formulation selection, manufacturing and regulatory filings (both those at the bench and their managers) will benefit from this course.

**TOPICS**

- ▶ General Considerations
  - A variety of potential reasons for dissolution testing
  - Regulatory requirements and compendia guidances
  - Identifying the design requirements for your particular method
- ▶ Dissolution Method Development Fundamentals
  - Apparatus: selection and qualification
  - Dissolution medium
  - Testing parameters: speed, sampling times
  - Measurement options: UV, HPLC, others
  - Interactive exercise on method development
- ▶ Evolution of Dissolution Methods
  - Early development: formulation selection
  - Late development: establishing specifications
  - Marketed products: post approval changes
- ▶ Correlating *In-Vitro* and *In-Vivo* Data
  - Bio-relevant dissolution
  - Comparing dissolution data to animal and human data
  - Different types of correlations
- ▶ Method Troubleshooting
  - Extensive presentation of common issues observed during method development and product lifecycle, and appropriate ways to diagnose and respond to issues
  - Discussion of issues observed by participants
- ▶ Course Review
  - Questions and answers

**ABOUT THE INSTRUCTOR**

**Mr. Gregory Martin** is President of Complectors Consulting, which provides consulting services and technical training related to pharmaceutical analysis, regulatory and compendial issues and improving lab efficiency. He has 30 years of experience in the pharmaceutical industry, including extensive responsibility for dissolution method development and troubleshooting, including 24 years in Research and Development for a major PhRMA company, where he was Director of Pharmaceutical Analytical Chemistry. He has particular interest in dissolution, and has made numerous presentations on dissolution method development and instrument calibration, HPLC method development and validation, and related substances including residual solvents. He has served on the USP Dissolution Project Teams and PhRMA Dissolution Expert Committee, and is currently Chair-elect for the AAPS In Vitro Release and Dissolution Testing Focus Group. He is also Vice Chair of the USP General Chapters (Physical Analysis) Expert Committee, where he has had significant impact on several General Chapters, including Residual Solvents, Validation of Analytical Procedures, Instrument Qualification and Chromatography, and Chair of the USP Expert Panel on Weights and Balances.

## Introduction to Metabolomics

**New One-Day Course E11-45, Thursday, November 17, 2011, 8:30am-5:30pm**

Mr. William R. Wikoff, University of California, Davis, CA

### **COURSE DESCRIPTION**

Metabolomics can be defined as the systems-level investigation of small molecules and metabolites in biological systems. The course will provide the scientist with an overview of the field, with an emphasis on practical, mass spectrometry-based approaches, presented in a clear scientific framework. The entire process of metabolomics, from study design, sample preparation and extraction, chromatography, mass spectrometry, data processing and analysis will be presented. Topic will include: types of detectors and their relative merits for specific metabolomics applications, ionization sources. Application of LC/MS and GC/MS, including a comparison of observable compounds in these techniques. A brief coverage of specialized instruments. Methods for sample extraction and chromatography will be covered in detail. Methods such as UPLC/UHPLC, targeted versus untargeted methods and lipidomics will be covered. Peak integration, data alignment, and software will be described in detail. Data analysis approaches will be discussed, including uni- and multi-variate statistics, with an emphasis on selecting straightforward approaches appropriate for a given problem. Basic statistics for metabolomics: types of t-tests, multiple testing correction, False Discovery Rate, basic multi-variate methods. Approaches to biomarker discovery; metabolomics in drug discovery. Review and discussion of selected publications from the literature (case studies). Some familiarity with mass spectrometry and analytical chemistry is preferred, but background will be provided.

### **WHO SHOULD ATTEND**

This one-day course will benefit anyone with an interest in learning approaches and methods for mass spectrometry-based metabolomics and metabolic profiling, including those in the pharmaceutical industry, academic and core laboratories, at all levels. It is intended to provide any introductory material necessary for understanding, although the ideal student will have basic mass spectrometry experience.

### **TOPICS**

- ▶ Introduction and Overview with Historical Background
- ▶ Mass Spectrometry
  - Instrumentation for metabolomics
  - Ionization methods
  - Review of mass analyzers
  - General instrumentation types for metabolomics: quadrupole, triple quad, ion trap, TOF, QTOF, FT-ICR, orbitraps, and other hybrid instruments
  - Discussion of relative merits and limitations for each approach
- ▶ Sample Preparation and Extraction
  - Methods specific for blood plasma, urine, and solid tissue, and others
- ▶ Design of the Experiment
  - Sampling and basic statistics
  - Designing experiments to determine analytical and biological variability
- ▶ Liquid Chromatography Approaches for Metabolomics
  - Basic reverse phase solvents and gradients for metabolomics
  - UHPLC in metabolomics
- Newer developments, including LC solutions for polar metabolites
- New chromatography approaches
- Compound Identification
- Basic identification of unknown compounds
- Minimum standards for compound identification
- Compound identifiers
- Correct reporting of IDs
- Compound and spectral libraries
- Available databases for metabolomics and chemometrics
- ▶ Data Post Processing and Analysis
  - Retention time alignment and data integration
  - Basic software options
  - New developments
  - Differences between LCMS and GCMS data processing
  - Evaluating the overall experiment
- ▶ Data Interpretation and Graphical Representation
  - Network models
  - Integration with other data types, including transcriptomics and proteomics

### **ABOUT THE INSTRUCTOR**

**Mr. William R. Wikoff** has a Ph.D. from Purdue University in Biophysics. He has been involved in metabolomics research for six years, with numerous publications in the field, and has focused on applying metabolomics, proteomics, and other systems biology approaches to understanding human health and disease. His current research interests include neurodegenerative diseases, human variation in the drug response (pharmacometabolomics) and the interaction between the gut microbiome and host. He is presently in the University of California's Davis Genome Center.

## Detection and Characterization of Drug Metabolites in Drug Discovery and Development

**New One-Day Course E11-46, Thursday, November 17, 2011, 8:30am-5:30pm**

Dr. Donglu Zhang, Bristol-Myers Squibb, Princeton, NJ

Dr. Mingshe Zhu, Bristol-Myers Squibb, Princeton, NJ

### COURSE DESCRIPTION

This one-day short course is designed for analytical chemists and 'new' drug metabolism scientists who would like to gain additional skills in metabolite detection and identification using advanced LC/MS and other analytical tools. The course provides an overview of current drug metabolism/disposition studies in the pharmaceutical industry, cutting-edge analytical technologies for metabolite detection, identification and quantification, and their applications to drug discovery and development with case studies.

### WHO SHOULD ATTEND

Analytical chemists and drug-metabolism scientists and others interested in analytical chemistry in drug discovery and development.

### TOPICS

- ▶ Basics of Drug Disposition and Metabolism
  - Drug disposition: ADME
  - Biotransformation reactions: Phase I and II reactions/bioactivation pathways
  - Metabolizing enzymes
  - Common analytical techniques
- ▶ LC/MS Technologies for Metabolite Detection and Identification
  - Triple quadrupole MS
  - Ion trap MS
  - Triple quadrupole-linear ion trap MS (Q-trap)
- High resolution MS (Orbitrap)
- MS data mining technologies
- ▶ Metabolite Identification in Drug Discovery
  - In vitro metabolism models
  - Metabolic soft spot determination
  - Reactive metabolite screening
- ▶ Metabolic Profiling and Identification in Drug Development
  - Role of drug metabolism in drug development
  - Plasma metabolite profiling in the first in human studies
  - Radiolabeled ADME study

### ABOUT THE INSTRUCTORS

**Dr. Donglu Zhang** received his Ph.D. in Bioorganic Chemistry (Dr. C. Dale Poulter) from the University of Utah. He had three years of postdoctoral training in enzyme mechanism/kinetics before working in the National Center for Toxicological Research of FDA to develop metabolite-generating microbial bioreactors (Dr. Carl E Cerniglia). He has been working at Bristol-Myers Squibb since 1997. His current research interests include investigative metabolism, metabolite detection, identification, and quantification, drug metabolism enzymology, LC/MS methodologies, and their applications to drug discovery and development. He has published >65 peer-reviewed articles and book chapters, and co-authored the book of "Drug Metabolism in Drug Design and Development: Basic Concepts and Practice" in 2007. Dr. Zhang is a recipient of the Ondetti & Cushman Award on co-invention of the mass-defect filtering technology, the highest scientific recognition at Bristol-Myers Squibb. He has been teaching drug metabolism short courses at ACS meetings and EAS Symposia. Contact information: Phone, 732-322-4200; email, donglu.zhang@bms.com.

**Dr. Mingshe Zhu** is a Principal Scientist in the Department of Biotransformation, Pharmaceutical Candidate Optimization, Bristol-Myers Squibb, Princeton, NJ, USA. He has over 12 years of experience in drug discovery, development and registration. His research interests include lead optimization via DMPK approaches, regulatory drug metabolism, CYP-mediated bioactivation and applications of new LC/MS and radiodetection techniques to ADME studies. Recently, his group has focused on DMPK supports to discovery and development programs and the development of new analytical technology, such as high resolution mass spectrometry/mass defect filtering and linear ion trap mass spectrometry for drug metabolite identification. Dr. Zhu received BS in Biochemistry and MS in Chemistry. He completed his Ph.D. training in analytical toxicology at SUNY at Albany, and post-doctoral fellowship in drug metabolism at University of Washington. Dr. Zhu is frequently invited to speak at conferences, society meetings and symposiums on drug metabolism and LC/MS technology. He often teaches drug metabolism short courses at American Chemistry Society meetings and Eastern Analytical Symposia. Dr. Zhu is a recipient of the Ondetti & Cushman Award, one of the highest scientific awards at Bristol-Myers Squibb. He has published over 50 research articles including several book chapters and co-authored the book of "Drug Metabolism in Drug Design and Development: Basic Concepts and Practice" in 2007.

## The Chemistry of Drug Degradation

**One-Day Course E11-47, Thursday, November 17, 2011, 8:30am-5:30pm**

Dr. Karen Alsante, Pfizer Global Research & Development, Groton, CT

### COURSE DESCRIPTION

This workshop is designed to provide participants with an in depth of knowledge of the chemical reactions involved in the most common degradation pathways of drugs.

The Chemistry of Drug Degradation: This topic will be covered by carefully examining the major mechanisms of chemical decomposition of pharmaceuticals in the context of common functional groups. The major mechanisms of chemical decomposition of pharmaceuticals include hydrolysis/dehydration, oxidation, isomerization/ epimerization, decarboxylation, dimerization/ polymerization, cyclization, rearrangements, photolysis, and transformation products involving reaction with excipients or counterions(salt forms). Real world examples will be given to illustrate many of the degradation mechanisms.

- Identifying critical molecular structures
- Which structures are likely to react?
- Predicting the likely degradation products
- Interactive problem solving session
- Developing degradation mechanisms
- Relating the chemistry to ICH guidelines

### WHO SHOULD ATTEND

This one-day course will benefit analysts and formulators who develop methods and formulations, perform forced degradation and structure elucidation of impurities and degradants of pharmaceutical products. To get the most out of the course, we highly recommended that you have at least two years of pharmaceutical analysis or drug development experience.

### TOPICS

- ▶ Introductions
- ▶ General considerations
- ▶ Main degradation pathways
- ▶ Functional Groups, Drug-Excipient Reactions, and Examples
- ▶ Carbonyl chemistry:
  - Esters, Lactones
  - Carboxylic acids
  - Ketones, Aldehydes
  - Amides, Lactams
  - Carbamates
  - Imides
- ▶ Nitrogen functional groups:
  - Nitriles
  - Amines
  - Imines
  - Enamines
  - Nitro groups
- ▶ Ethers, thioethers, and sulfonyl chemistry:
  - Ethers, thioethers
  - Sulfonamides, sulfonylureas
  - Epoxides
- ▶ Alkyl halides/hydroxyls:
  - Alkyl halides
  - Hydroxyls, thiols, phenols
- ▶ Conjugated Double Bond Systems:
  - Benzyl groups
  - Olefins, allylic groups
- ▶ Additional Reactions:
  - Epimerization, dimerization
  - Ring transformations
  - Cis/trans isomerization
- ▶ Prediction

### ABOUT THE INSTRUCTOR

**Dr. Karen Alsante** is an Associate Director in Research Analytical at Pfizer Global Research and Development: Groton, CT. Dr. Alsante received a BA with honors in chemistry from HolyCrossCollege in 1989 and her PhD in organic chemistry from DukeUniversity in 1994. Dr. Alsante started at Pfizer in 1994 as a development scientist in Groton Quality Operations. In 1997, Dr. Alsante developed a Degradation Group in Analytical R&D responsible for gaining a better understanding of drug substance and drug product chemical and physical stability. In July 2004, Dr. Alsante shifted to group leader of a new Solid State Characterization group within Analytical R&D focused on crystalline/amorphous/polymorph content, particle size/morphology and particulate analysis. In January 2006, Dr. Alsante began her current position as a Research Fellow for Research Analytical focused on early analytical research activities starting in partnership with Discovery and progressing through development to Phase 2 clinical trials.