

## Curriculum Vitae (2017-07-05)



### Peter de Boves Harrington

Center for Intelligent Chemical Instrumentation  
Department of Chemistry and Biochemistry  
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WWW: <http://www.ohio.edu/chemistry/harrington/index.cfm>

### Education

Ph.D. (Analytical Chemistry), University of North Carolina, Chapel Hill, NC, 1988  
Dissertation Advisor, Thomas L. Isenhour

B.S. (Chemistry), Randolph-Macon College, Ashland, VA, 1980

### Professional Experience

CannaPrint, Board of Advisors, 2016-2017

Director of the Forensic Chemistry Programs, 2012-2015

Visiting Scholar, Universitetet i Agder, Kristiansand, NO, August, 2010.

Director of the Master of Science Program in Forensic Chemistry, 2009-2015

Chercheur Etranger, Université Paul Cézanne, Marseille, FR September-December, 2008.

Summer Visiting Fellow (ORISE) Food and Drug Administration/Center for Food Safety and Applied Nutrition, MD, June-August, 2007

Summer Visiting Fellow (Contractor) National Institutes of Health/National Institute of Mental Health, Bethesda, MD, July-August, 2005

Director of the Forensic Chemistry Program, 2004-2009

Professor, Ohio University, 2004-Present

Summer Visiting Fellow (Contractor) National Institutes of Health/National Institute of Child Health and Human Development, Bethesda, MD, July-August, 2004

Summer Faculty Fellow, Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID, June-July, 2003

Director, Ohio University Center for Intelligent Chemical Instrumentation, 2002-

Present

Faculty Fellow, Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID, 2001-2002

Associate Professor, Ohio University, 1995-2004 (Tenured 1995)

Adjunct Professor Environmental Science, Ohio University, 1994-Present

Assistant Professor, Ohio University, 1989-1995

Research Assistant Professor, The Colorado School of Mines, Golden, CO, 1988-1989

Research Associate, The Colorado School of Mines, Golden, CO, 1987-1988

Flavor Chemist, Nabisco Brands Inc., Wilton, CT, 1980-1982

**Research Interests**

Intelligent analytical instrumentation, chemometrics, microscale sensors, ion mobility and mass spectrometries, automated and online decision-making, pattern recognition, artificial intelligence and novel representations of chemical information. Successful developments include fuzzy rule-building expert systems, temperature-constrained neural networks, analysis of variance – principal component analysis (ANOVA-PCA), generalized sensitivity analysis of neural networks, two-dimensional wavelet compression and modeling of sensor data, and the Latin-partition bootstrap method for statistically evaluating classifiers.

**Teaching Interests**

Analytical chemistry presented as a unified set of principles for ascertaining chemical information. Development of instructional microanalytical experiments and computer enhanced learning methods, including web-based learning and virtual instrumentation.

**Courses Taught**

Graduate Level:

Chemometrics  
Advanced Analytical Spectroscopy  
Advanced Analytical Separations  
Analytical Review

Dual Level:

Arson and Explosives  
Chemical Separation Methods  
Chemical Separation Methods Lab  
Spectrochemical Analysis  
Spectrochemical Analysis Lab  
Forensic Chemistry 1  
Forensic Chemistry 2  
Forensic Chemistry Laboratory 1  
Forensic Chemistry Laboratory 2

Undergraduate Level:

Quantitative Analysis  
Quantitative Analysis Lab

## Fundamentals of Chemistry III

**Research Group**

Xinyi Wang	(Ph.D. 2017)
Ahmet Aloglu	(Ph.D. 2018)
Xue Zhao	(M.S. 2017)

**Alumni**

Ryan O'Donnell	(B.S. 2009)
Danielle Melaragno	(B.S. 2007)
Abby Burg	(B.S. 2006)
Leanna Ergin	(B.S. 2006)
Lisa Stout	(B.S. 2006)
Betsy Gombas	(B.S. 2004)
Nicole Burrow	(B.S. 2003)
Jennifer Cline	(B.S. 2003)
Yuka Minoshima	(B.S. 2002)
Erin Kolbrich	(B.S. 2002)
Morgan Patchett	(B.S. 2001)
Jeanette Perr	(B.S. 2001)
Aaron Mehay	(B.S. 2001)
Aaron Urbas	(B.S. 2001)
Lisa Shaw	(B.S. 2000)
Jennifer Mueller	(B.S. 1998)
Jay Stotz	(B.S. 1998)
Eric Reese	(B.S. 1997)
Joshua Siegel	(B.S. 1993)
Hans Whittenburg	(B.S. 1992)
Brian Pack	(B.S. 1992)
Alan Hendricker	(B.S. 1992)

**MS**

- George Bota, "Direct Detection of Trimethylamine in Meat Food Products Using Ion Mobility Spectrometry" (MS 2005).
- Matt Rainsberg, "Thermal Desorption Solid-Phase Microextraction Inlet for Differential Mobility Spectrometry" (MS 2005).
- Susan Slagel, "Development of a Wireless Data Transmission System for a Handheld Chemical Sensor" (MS 1999).
- Eric Reese, "The Analysis of Methamphetamine Hydrochloride by Thermal Desorption Ion Mobility Spectrometry and SIMPLISMA" (MS 1998).
- Hailing Yin, "Quantitative Analysis of Formaldehyde in Air Using Ion Mobility Spectrometry" (MSES 1997).
- Deborah Wuersig, "Quantitative Spectra-Retention Relationships" (MS 1994).

**PhD**

- Mengliang Zhang, "Determination of Environmental Pollutants by Gas Chromatography/Mass Spectrometry with Chemometrics (PhD 2014).
- Ayat H. Bani Rashaid, "Clinical and Forensic Biomarkers in Human Hair" (PhD 2014).
- Zhengfang Wang, "Thiol Protein/Peptide Modification by *N*-(Phenylseleno)phthalimide and Applications of Chemometrics in Organic Food Authentication" (PhD 2014).
- Zhanfeng Xu, "Prediction and Classification of Physical Properties by Near-Infrared Spectroscopy and Baseline Correction of Gas Chromatography Mass Spectrometry Data of Jet Fuels by Using Chemometric Algorithms" (PhD 2012).
- Xiaobo Sun, "Forensic Applications of Gas Chromatography/Mass Spectrometry, High Performance Liquid Chromatography—Mass Spectrometry and Desorption Electrospray Ionization Mass Spectrometry with Chemometric Analysis" (PhD 2012).
- Weiyang Lu, "Development of Radial Basis Function Cascade Correlation Networks and Applications of Chemometric Techniques for Hyphenated Chromatography—Mass Spectrometry Analysis" (PhD 2011).
- Yao Lu, "Forensic Applications of Gas Chromatography—Differential Mobility Spectrometry, Gas Chromatography/Mass Spectrometry, and Ion Mobility Spectrometry with Chemometric Analysis" (PhD 2010).
- Ping Chen, "Applications of Chemometric Algorithms to Ion Mobility Spectrometry and Matrix Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry" (PhD 2008).
- Preshious Rearden, "Applications of Solid Phase Microextraction with Ion and Differential Mobility Spectrometry for the Study of Jet Fuels and Organophosphonates" (PhD 2006).
- Mariela L. Ochoa, "Forensic and Proteomic Applications Of Thermal Desorption Ion Mobility Spectrometry and Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry" (PhD 2005).
- Libo Cao, "Nonlinear Wavelet Compression Methods for Ion Analyses and Dynamic Modeling of Complex Systems" (PhD 2004).
- Guoxiang Chen, "Real-Time Wavelet Compression and Self-Modeling Curve Resolution for Ion Mobility Spectrometry" (PhD 2003).
- Tricia L. Buxton, "Solving Problems in Ion Mobility Measurements of Forensic Samples with Thermal Desorption and Dynamic Modeling" (PhD 2002).
- Paul Rauch "Making a Smart Instrument: Chemometric Methods Applied to Ion Mobility Spectrometry for Pattern Recognition and Feature Extraction" (PhD 2000).
- Chuanhao Wan "Analysis of Aromatic Compounds in Water by Ion Mobility Spectrometry and Classification of Pesticides and Bacteria Using Artificial Neural Networks and Mass Spectrometry" (PhD 1999).
- Chunsheng Cai "Application of Wavelet Transform and Cascade Correlation Neural Networks to Mass and Ion Mobility Spectrometry" (PhD 1999).

Lijuan Hu "Development of Chemometric Tools for Chromatograms and Ion Mobility Spectra" (PhD 1997).

Peter J. Tandler "The Application and Development of Chemometric Methods for the Analysis of Plastic Recycling and Mo(CO)<sub>6</sub> Photodecomposition Data" (PhD 1997).

Peng Zheng "Application of Chemometric Tools for Ion Analysis in Time of Flight Secondary Ion Mass Spectrometry and Ion Mobility Spectrometry" (PhD 1996).

Busolo Wa Wabuye "Application of Associative Memories for Background Correction of Spectra" (PhD 1995).

### **Visiting Scholars**

Rico Warias, "Detection of Dopamine and Serotonin in Bananas", Universität Leipzig, Germany (1/Sep/2014-15/Dec/2014).

Cevdet Demir, "Application of Chemometrics to the Study of Polyphenols in Honey by HPLC", Uludağ Üniversitesi, Bursa, Turkey (24/Jun/2013-31/Aug/2013).

Liu Jin, "Application of Differential Mobility Spectrometry to the Detection of Explosive Taggants", Chinese Peoples Public Security University, Beijing, PRC, (1/Dec/2010-31/Nov/2011).

Haining Wang, "Knowledge Acquisition for the Prediction of Large-scale Group Events", Chinese Peoples Public Security University, Beijing, People's Republic of China, (1/Dec/2010-31/Nov/2011).

Alfred Christy, "Vibrational Spectroscopy of Biological Fluids", Agder University College, Kristiansand, Norway (1/Feb/2008-1/Jul/2008).

Ornella Smilla, "MALDI-MS of Gram Positive Bacteria", Université Paris 7 - Denis-Diderot, France (24/Apr/2005-1/Jul/2005).

Corinna Sykora, "MALDI-MS of Surfactants and Bacteria", Universität Leipzig, Germany (1/Apr/2003-1/Jul/2003).

Zhuoyong Zhang, "Neural Networks Applied to Mass Spectrometric Analysis of Bacteria", North East Normal University, Changchun, PRC (12/Sep/2000-15/Dec/2000).

### **Awards and Recognition**

*Analytix* (Editorial Advisory Board, 2017-)

*Investigative Forensic Sciences* (Editor, 2016-)

*Journal of Analysis and Testing* (Editorial Advisory Board, 2016-)

Ohio University College of Arts & Sciences Outstanding Faculty Research Award (2016)

*Nature: Scientific Reports* (Editorial Board Member 2015-)

Fellow of the American Academy of Forensic Sciences (2015-)

*International Journal of Spectroscopy* (Editor, 2007-2017).

Award for Academic Achievement, North East Normal University, Changchun, PRC, December 7, 2006.

Research Opportunity Award, The Research Corporation 2001-2003.

Appointed Visiting Professor at North East Normal University, Changchun, PRC, 2001.

*Analytica Chimica Acta* (Editorial Advisory Board, 1997-2000)

*Analytica Chimica Acta* (Editorial Advisory Board, 2003-2005)

*Chemometrics and Intelligent Laboratory Instruments* (Editorial Advisory Board, 1991-)

*Critical Reviews in Analytical Chemistry* (Editorial Advisory Board, 2013-)

*Journal of Spectroscopy and Dynamics* (2010-)

*Talanta* (Editorial Advisory Board, 2005-2010)

*Analytical Sciences Digital Library* (Contributing Editor 2003-2005)

"The Future of Spectroscopy: Bright Young Stars" *Spectroscopy*, October 1995, 60.

### **Peer Review Participation**

#### **Working Groups**

US Pharmacopeia Chemometrics Panel of Experts, September 27, 2013-present.

US Pharmacopeia Skim Milk Powder Advisory Group, Chemometrics and Statistics Sub-team, June 18, 2012-present.

AOAC Expert Review Panel Guidelines for Validation of Botanical Identification Methods, April 14, 2011-present.

AOAC Working Group: Validation of Botanical Identification Methods 2010.

**Proposal**

Battelle, Program Review, Columbus, OH, February 1, 2005.

Department of Defense Experimental Program to Stimulate Competitive Research (DEPSCoR).

Department of Homeland Security, NA-22 Site Review  
Oak Ridge National Laboratory, Micro-ITMS, Oak Ridge, TN, November 17, 2005.  
Oak Ridge National Laboratory, Micro-IMS, Oak Ridge, TN, April 20, 2004.

Department of Homeland Security, Secret Review Panel  
Washington, DC, August 27-28, 2007 (4).

International Science and Technology Center (ISTC)

National Aeronautics and Space Administration

National Defense Science and Engineering Graduate Fellowship  
Review Panel, Online Review, February 21, 2014  
Review Panel, Washington, DC, February 20, 2010  
Review Panel, Washington, DC, February 21, 2009  
Review Panel, Washington, DC, February 17, 2008  
Review Panel, Washington, DC, February 18, 2006  
Review Panel, Washington, DC, February 19, 2005  
Review Panel, Washington, DC, February 27, 2004  
Review Panel, Washington, DC, February 22, 2003  
Review Panel, Washington, DC, February 23, 2002  
Review Panel, Research Triangle Park, NC, February 7-8, 1998  
Review Panel, Research Triangle Park, NC, February 8-9, 1997  
Review Panel, Research Triangle Park, NC, February 11-12, 1995

National Institutes of Health  
Special Study Section *Fungal Diagnostics*, D.C. June 18-19, 2009 (6).  
Special Study Section *Computational Biology*, D.C. October 31-November 01, 2002 (7)  
Special Study Section Reverse Site Visit, Tyson's Corners, VA, Apr. 21-22, 1994

National Institute of Justice  
R&D in Forensic Science for Criminal Justice Purposes, Standing Review Panel  
Impression and Trace Evidence, Arlington, VA, June 16-17, 2014 (4).

R&D in Forensic Science for Criminal Justice Purposes, Standing Review Panel  
Impression and Trace Evidence, Arlington, VA, June 11-12, 2015 (6).  
R&D in Forensic Science for Criminal Justice Purposes, Standing Review Panel  
Impression and Trace Evidence, Arlington, VA, June 13-14, 2016 (4).

National Science Foundation

SBIR Review Panel, Arlington, VA, February 15, 2007 (8)  
CCLI Review Panel, Arlington, VA, February 4-6, 2004 (12)  
CCLI-A&I Review Panel, Arlington, VA, Jul. 23-26, 2001 (12)  
CCLI-A&I Review Panel, Arlington, VA, February 17-20, 1999 (13)  
ILI Review Panel, Arlington, VA, January 21-24, 1998 (19)  
SBIR Review Panel, Arlington, VA, September 28-29, 1995  
SBIR Review Panel, Arlington, VA, September 5-6, 1994

Natural Sciences and Engineering Research Council of Canada

Research Corporation

University of Ontario Institute of Technology Bachelor of Science in Forensic  
Chemistry, Postsecondary Education Quality Assurance Board, Site visit  
Oshawa, January 31, 2005.

U.S. Civilian Research and Development Foundation

**Manuscript**

*Analytical Chemistry*  
*Analytica Chimica Acta*  
*Applied Spectroscopy*  
*Biotechnology and Bioengineering*  
*Chemometrics and Intelligent Laboratory Instruments*  
*Environmental Science and Technology*  
*Field Analytical Chemistry and Technology*  
*Fresenius Journal of Analytical Chemistry*  
*IEEE Vision, Image and Signal Processing*  
*International Journal of Forensic Sciences*  
*Journal of Analytical and Applied Pyrolysis*  
*Journal of the American Society of Mass Spectrometry*  
*Journal of Chemometrics*  
*Journal of Chemical Education*  
*Journal of Forensic Sciences*  
*Lung*  
*Mikrochimica Acta*  
*Nature*  
*PLOS ONE*  
*Spectroscopy*



*Talanta*  
*Vibrational Spectroscopy*

### **Professional Affiliations**

American Academy of Forensic Sciences (Criminalistics, 2008-)  
Fellow, 2015-  
Commissioner, Forensic Science Education Programs Accreditation Commission  
(FEPAC), 2008-2009.  
American Chemical Society (1980-2009)  
Forensic Science Institute of Ohio  
International Chemometrics Society  
International Society for Ion Mobility Spectrometry  
Steering Committee (2005-2007)  
Secretary (2006-2007)  
International Forensic Science Education Consortium  
New York Academy of Sciences (Lifetime Member)  
North American Academy of Arts & Sciences Fellow (Lifetime Member)  
Society for Analytical Chemists of Pittsburgh (Lifetime Member)  
Society for Applied Spectroscopy  
Sigma Xi **Secretary** (2012-present)  
Local Section Ohio University, Athens, OH  
  
Sigma Xi **President** (2005-2012)  
Local Section Ohio University, Athens, OH

### **Scientific Committee**

The 16<sup>th</sup> Chemometrics in Analytical Chemistry, Barcelona, Spain, June 6-10, 2016.  
  
The 15<sup>th</sup> Chemometrics in Analytical Chemistry, Changsha, China, June 22-26,  
2015.  
  
The 2<sup>nd</sup> International Symposium on Profiling 2015 (ISPROF-2015), Caparica,  
Portugal, September 21-24, 2015.  
  
The 1<sup>st</sup> International Symposium on Profiling 2013 (ISPROF-2013), Caparica,  
Portugal, September 2-4, 2013.  
  
The 3<sup>rd</sup> Symposium on Computer Applications and Chemometrics in Analytical  
Chemistry, Lake Balaton, Hungary, July 3-7, 2006.

### **Program and Organizing Committee**

*Chemometrics Section Chair*, The Federation of Analytical Chemistry and  
Spectroscopy Societies, SciX 2017, October 8-13, 2017, Reno, NV.

*Chemometrics Section Chair*, The Federation of Analytical Chemistry and

Spectroscopy Societies, SciX 2016, September 18-23, 2016, Minneapolis, MN.

*Chemometrics Section Chair*, The Federation of Analytical Chemistry and Spectroscopy Societies, SciX 2015, September 27-Oct 2, 2015, Providence, RI.

The 2<sup>nd</sup> International Symposium on Profiling 2015 (ISPROF-2015), Caparica, Portugal, September 21-23, 2015, Scientific Committee.

The 1<sup>st</sup> International Symposium on Profiling 2013 (ISPROF-2013), Caparica, Portugal, September 2-4, 2013, Scientific Committee.

6th Shanghai International Symposium on Analytical Chemistry, Shanghai, China, October 16-18, 2012.

The 15<sup>th</sup> International Conference on Ion Mobility Spectrometry, July 23-27, 2006, Honolulu, HI.

The 14<sup>th</sup> International Conference on Ion Mobility Spectrometry, July 24-28, 2005, Maffliers, France.

The 13<sup>th</sup> International Conference on Ion Mobility Spectrometry, July 25-29, 2004, Gatlinburg, TN.

Ohio Analytical Chemistry Consortium, 2005, Columbus, OH.

Ohio Analytical Chemistry Consortium, 2004, Columbus, OH.

Ohio Analytical Chemistry Consortium, 2003, Columbus, OH.

Ohio Analytical Chemistry Consortium, 2002, Columbus, OH.

Chemometrics and Analytical Chemistry 2002, Seattle, WA.

Ohio Aerospace Institute Neural Networks Symposium and Workshop 1995  
Athens, OH, August 21-22.

### **Symposium Organizer/Presider**

*Session 3 Chromatographic Analysis*, International Congress on Analytical Sciences 2017, May 7, 2017, Haikou, China.

*Chemometrics*, 5<sup>th</sup> Annual Congress of Analytix 2017, March 23, 2017, Fukuoka, Japan.

*New Frontiers in Chemometrics*, The Federation of Analytical Chemistry and Spectroscopy Societies SciX 2016, September 19, 2016, Minneapolis, MN,  
**Organized.**

*Omics and Forensics*, Chemometrics in Analytical Chemistry 2016, June 8, 2016,

Barcelona, Spain.

*Beyond PCA and PLS: New Frontiers in Chemometrics*, The Federation of Analytical Chemistry and Spectroscopy Societies SciX 2015, September 28, 2015, Providence, RI, **Organized**.

*Chemometrics and Experimental Design*, The Federation of Analytical Chemistry and Spectroscopy Societies SciX 2015, October 1, 2015, Providence, RI, **Organized**.

*Criminalistics: The Trasks and Hamiltons Consider More Criminalistics Topics*, The 67<sup>th</sup> American Academy of Forensic Sciences Annual Meeting, February 19, 2015, Orlando, FL.

*Criminalistics: Applications of Forensic Science*, The 66<sup>th</sup> American Academy of Forensic Sciences Annual Meeting, February 22, 2014, Seattle, WA.

*Final Session*, The 1<sup>st</sup> International Symposium on Profiling 2013 (ISPROF-2013), September 4, 2013, Caparica, Portugal.

*Fuzzy Algorithms for the Development of Intelligent Chemical Instrumentation*, The 2009 Sixth International Conference on Fuzzy Systems and Knowledge Discovery, August 15, 2009, Tianjin, PRC, **Organized**.

*Invited Fuzzy Algorithms and Applications: Fuzzy Data Analysis*, The 2009 Sixth International Conference on Fuzzy Systems and Knowledge Discovery, August 16, 2009, Tianjin, PRC.

*Chemometrics*, the 59<sup>th</sup> Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), March 6, 2008, New Orleans, LA.

*Chemometrics*, the 58<sup>th</sup> Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2007), February 27, 2007, Chicago, IL.

*Ion Mobility Spectrometry*, American Academy of Forensic Science 59<sup>th</sup> Annual Meeting, February 24, 2007, San Antonio, TX, **Organized**.

*Modeling*, The 15<sup>th</sup> International Conference on Ion Mobility Spectrometry, July 25, 2006, Honolulu, HI.

The 3<sup>rd</sup> Symposium on Computer Applications and Chemometrics in Analytical Chemistry, Chair for Plenary Session, Lake Balaton, Hungary, July 6, 2006.

*Pitfalls and Potentials of Generalized Two-Dimensional Correlation Spectroscopy*,

The 57<sup>th</sup> Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, Orlando, FL, March 13, 2006.

*Sampling and Calibration for Explosives*, The 14<sup>th</sup> International Conference on Ion Mobility Spectrometry, Maffliers, France, July 25, 2005.

*Instrumentation*, The 13<sup>th</sup> International Conference on Ion Mobility Spectrometry, Gatlinburg, TN, July 28, 2004.

*Ionization and Reactant Ions*, The 12<sup>th</sup> International Conference on Ion Mobility Spectrometry, Umeå, Sweden, July 28, 2003.

*Bioanalytical Applications of Chemometrics*, Chemometrics in Analytical Chemistry, 2002, Seattle, WA, September, 2002. **Organized.**

*Chemometrics in the Next Millennium*, The 2000 Federation of Analytical Chemistry and Spectroscopy Societies Conference, Nashville, TN, September 2000. **Organized.**

*Computational Methods I*, The 1998 Federation of Analytical Chemistry and Spectroscopy Societies Conference, Austin, TX, October, 1998.

*Real World Analysis II*, The 1997 Federation of Analytical Chemistry and Spectroscopy Societies Conference, Providence, RI, October, 1997.

*Chemometric Applications Using ICP-AES, ICP-MS, and GC-MS Techniques*, The 1996 Federation of Analytical Chemistry and Spectroscopy Societies Conference, Kansas City, MO, October, 1996.

Chemometrics in Analytical Chemistry 96, Tarragona, Spain, June, 1996.

*Near Infrared Spectroscopy for Biomedical Sciences and Biotechnology*, The 1995 Federation of Analytical Chemistry and Spectroscopy Societies Conference, Cincinnati, OH, October 1995.

*Making the Connection: Neural Networks and Chemistry*, The 1994 Federation of Analytical Chemistry and Spectroscopy Societies Conference, St. Louis, MO, October 1994. **Organized**

*Chemometrics II*, The 1994 Pittsburgh Conference, Chicago, IL, March 1994, **785-794.**

*Capillary Electrophoresis: Characterization of Proteins and Peptides*, The 1992 Pittsburgh Conference, New Orleans, LA, March, 1992, **365-374.**

Chemometrics in Analytical Chemistry-1992, Montreal, Quebec, Canada, July 17,

Session 7A.

COMPANA '92, Computer Application in Analytical Chemistry, Jena, Germany, August 24, Afternoon Plenary Session

### **Plenary Lectures**

P.B. Harrington, "Bootstrapping as a Tool to Automate Chemometric Methods", *Chiométrie XVIII 2017*, Paris, France, January 30, 2017, **PL-1**.

P.B. Harrington, "Fuzzy Optimal Associate Memories for Modeling Chemical Profiles: Authentication of Foods and Nutraceuticals", *The 1<sup>st</sup> International Symposium on Profiling 2013 (ISPROF-2013)*, Caparica, Portugal, September 3, 2013, **PL-4**.

P.B. Harrington, "Fuzzy Optimal Associative Memories for the Authentication of Nutraceuticals by Mass Spectrometry", *The 6<sup>th</sup> Shanghai International Symposium on Analytical Chemistry*, Shanghai, PRC, October 16, 2012.

P.B. Harrington, "Chemometric Opportunities in Proteomic Biomarker Discovery via Mass Spectrometry", *Fudan University Institutes of Biomedical Sciences Proteomics Pre-Conference*, Shanghai, PRC, September 22, 2007.

P.B. Harrington and Yao Lu, "Forensic Applications of Chemometrics: Classification of Accelerants from Fire Debris by Gas Chromatography-Differential Mobility Spectrometry (GC-DMS)", presented at the *10<sup>th</sup> International Conference on Chemometrics in Analytical Chemistry (CAC-2006)*, Aguas de Lindòia, Brazil, September 12, 2006.

P.B. Harrington, "Chemometric Opportunities in Proteomic Biomarker Discovery via Mass Spectrometry", presented at the *3<sup>rd</sup> Symposium on Computer Applications and Chemometrics in Analytical Chemistry (SCAC-2006)*, Lake Balaton, Hungary, July 5, 2006.

P.B. Harrington, P. Chen, and M.L. Ochoa, "Fuzzy Entropy Classification Systems and Their Application to Mass Spectrometry of the Proteome", *Mathematical Biosciences Institute Workshop 3 Computational Proteomics and Mass Spectrometry*, Columbus, OH, January 11, 2005.

A.L. Yergey, P.B. Harrington, N.E. Vieira, and R. Romero, "Mass Spectrometric Profiling for Disease Diagnosis: Development of Methodology", *Mathematical Biosciences Institute Workshop 3 Computational Proteomics and Mass Spectrometry*, Columbus, OH, January 11, 2005.

P.B. Harrington, M.L. Ochoa, N.E. Vieira, and A.L. Yergey, "Chemometric Approaches to Mass Spectrometry of the Proteome", *International Conference on Chemometrics and Bioinformatics in Asia (CCBA-2004)*, Shanghai China, October 16, 2004.

P.B. Harrington, "Minimal Neural Networks," Compana-1992, Jena, Germany, August 25, 1992.

### **Workshops and Training**

John Schmieding, "Mediation Training", OHIO University HDL, Athens, OH, 45701, June 6, 2007.

David M. Benjamin, PhD, "Testifying as an Expert in Court", The Franklin County Coroner's Office, Columbus, OH, June 30, 2006.

Larry R. Tate, MD, "Fire, Explosions and Death...An Update", Ohio Department of Transportation, Columbus, OH, October 4, 2006.

### **Research Support**

#### **Current (Co-PIs not listed)**

Source: US Department of Agriculture

Project Title: Algorithm Development and Support for Chemical Profiling of Botanicals and Foods

Investigator: Peter Harrington

Amount Funded: \$30,000

Period: 1/Oct/2016-09/31/2017

Source: US Department of Agriculture

Project Title: USDA ARS Post Doctorate

Investigator: Peter Harrington

Amount Funded: \$83,000

Period: 1/Apr/2015-09/31/2016

Source: Cannaprint, Inc.

Project Title: Profiling Botanical Products by NMR and MS

Investigator: Peter Harrington

Amount Funded: \$107,814

Period: 1/1/2016-12/31/2016

Source: Department of Energy

Project Title: Biomass Electrochemical Reactor for Upgrading Biorefinery Waste to Industrial Chemicals and Hydrogen

Investigator: John Staser

Amount Funded: \$1,840,914

Period: 3/1/2016-2/28/2019

Source: National Science Foundation

Project Title: MRI: Acquisition of a high resolution Orbitrap Q-Exactive Plus LC-

MS/MS system for enhancing research and education  
Investigator: Stephen Bergmeier  
Amount Funded: \$534,183  
Period: 1/Sep/2014-31/Aug/2017

**Past**

Source: US Department of Agriculture  
Project Title: Pattern Recognition for Food and Supplements  
Investigator: Peter Harrington  
Amount Funded: \$60,000  
Period: 15/Sep/2008-30/Sep/2011

Source: Marshall University/National Institutes of Justice  
Project Title: Data Analysis of Fuels  
Investigator: Peter Harrington  
Amount Funded: \$15,000  
Period: 1/Jun/10-31/Dec/10

Source: Marshall University/National Institutes of Justice  
Project Title: Data Analysis of Fuels  
Investigator: Peter Harrington  
Amount Funded: \$9,100  
Period: 1/Sep/09-31/Mar/10

Source: US Department of Agriculture  
Project Title: Pattern Recognition for Food and Supplements  
Investigator: Peter Harrington  
Amount Funded: \$23,600  
Period: 15/Sep/08-31/Jun/10

Source: Ohio University Growth Fund  
Project Title: Master of Science Program in Forensic Chemistry  
Investigator: Peter Harrington  
Amount Funded: \$147,358  
Period: 2007-2010

Supporting Agency: INSSI  
Project Title: Chemometric Methods for Classification and Property Prediction of Jet Fuel  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$30,000  
Period: 1/Sep/06-31/Aug/07

Source: National Institutes of Health/National Institute of Mental Health  
Title: Equipment Donation Bruker Daltonics Autoflex MALDI-MS

Principal Investigator: Peter de B. Harrington  
Value: \$200,000

Source: Amgen  
Title: Equipment Donation Bran+LuebbeInfraProver II Near-Infrared  
spectrometer  
Principal Investigator: Peter de B. Harrington  
Value \$15,000

Source: Homeland Security Advanced Research Projects Agency /GeoCenters  
Title: Lightweight Autonomous Chemical Identification System  
Principal Investigator: Peter de B. Harrington  
Amount Requested: \$16,048  
Award Period: 01/Feb/05-31/Aug/05

Source: US Army/GeoCenters  
Title: Sensor Fusion  
Principal Investigator: Peter de B. Harrington  
Amount Requested: \$52,500  
Award Period: 01/Nov/04-31/Sep/06

Supporting Agency: INSSI  
Project Title: Chemometric Methods for Classification and Property Prediction of Jet  
Fuel  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$90,000  
Period: 1/Jan/04-31/Dec/06

Supporting Agency: Ion Track Instruments  
Project Title: Rapid Screening of Bacteria Using the Itemizer  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$40,000  
Period: 1/Sep/03-31/Aug/04

Supporting Agency: GeoCenters  
Project Title: Thermodynamic Modeling of Ion Mobility Data  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$45,025  
Period: 1/Sep/03-31/Sep/04

Supporting Agency: INEEL  
Project Title: Software for IMS Support  
Principal Investigator: Peter Harrington  
Amount Funded: \$2,000  
Period 1/Jun/03-30/Sep/03



Supporting Agency: GeoCenters  
Project Title: Real-Time Algorithms for Compressing and Processing Ion Spectra  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$45,000  
Period: 1/Jun/02-31/Sep/03

Supporting Agency: Ohio University  
Project Title: Biological Safety Level-2 Laboratory in Clip. 177A  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$4,000  
Period: 18/Aug/01 – 30/Jun/03

Supporting Agency: Ohio Board of Regents Investment Fund  
Project Title: Mass Spectrometry Consortium for Materials and Medical  
Research  
Principal Investigator: Bruce McCord,  
Amount Funded: \$184,930  
Period: 01/May/02-01/May/03

Supporting Agency: INNSSI  
Project Title: Chemometric Methods for Classification of Jet Fuel  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$40,000  
Period: 1/Jan/03-31/Dec/03

Supporting Agency: Research Corp.  
Project Title: Data Compression, Modeling, and Pattern Recognition of Static Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) Images  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$75,000  
Period: 1/Jun/00-1/Jun/03

Supporting Agency: GeoCenters  
Project Title: Real-Time Algorithms for Compressing and Processing Ion Mobility Spectra  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$38,418  
Period: 1/Jun/2000-1/Jun/2001

Supporting Agency: Ohio Board of Regents Investment Fund  
Project Title: A Center of Excellence for Surface and Thin Film Analysis  
Principal Investigator: Wim van Ooij  
Amount Funded: \$1,480,000  
Period: 1997-2002.

Supporting Agency: Ion Track  
Project Title: Drug and Explosive Analysis  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$40,000 donation of an Itemizer Ion Mobility Spectrometer  
Period: 2001

Supporting Agency: Federal Aviation Administration  
Project Title: Drug and Explosive Analysis  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$110,000 donation of 2 Barringer Ionscan 350 Ion Mobility Spectrometers  
Period: 1999

Supporting Agency: Ohio Board of Regents Investment Fund  
Project Title: Establishment of Micromachining Technology in Analytical Chemistry  
Principal Investigator: Gilbert Pacey  
Amount Funded: \$1,500,000  
Presentation Team: February 22, 1996  
Period: 1996-2001

Supporting Agency: Ohio University Technology Incentives Package  
Project Title: Conveying the Undergraduate Chemical Analysis Laboratory to the  
Multimedia Class Room and Beyond  
Amount Funded \$15,000  
Period 1-Mar-99 1-Mar-00

Supporting Agency: Ohio University 1804 Fund  
Project Title: Upgrade of a Data System for a Gas Chromatograph-Mass Spectrometer  
Amount Funded: \$12,000  
Period: 18/Aug/98 – 30/Jun/00

Supporting Agency: National Biscuit Company  
Project Title: On-line Flavor Monitoring  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$100,000 in donation of HP 5988 GC-MS  
Period: NA

Supporting Agency: Ohio University Recruitment and Program Development Funds  
Project Title: "Improvement of Graduate Recruitment"  
Amount Funded: \$5,000  
Period: 1/Oct/1999-1/Oct/2000

Supporting Agency: Battelle, Columbus

Project Title: Development of Software for Spectroscopic Measurements  
Principal Investigator: Peter B. Harrington  
Amount Funded \$10,000 (total costs)  
Period: Nov. 3, 1997 to July 1, 1998.

Supporting Agency: US Army ERDEC BAA  
Project Title: Development of an Intelligent Ion Mobility Spectrometer for  
Counternarcotics Operations  
Principal Investigator: Peter B. Harrington  
Amount Funded \$200,000 (total costs)  
Period: June 1, 1995 to June 1, 1997

Supporting Agency: Battelle, Columbus  
Project Title: Development of Intelligent Algorithms for Apple Analysis  
Principal Investigator: Peter B. Harrington & Gary W. Small  
Amount Funded \$50,000 (total costs)  
Period: July 1, 1994 to July 1, 1995.

Supporting Agency: Battelle, RTP NC  
Project Title: Evaluation of Mass Spectral Identification Algorithms  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$50,295  
Period: August 8, 1993 to March 31, 1993

Supporting Agency: National Biscuit Company  
Project Title: On-line Flavor Monitoring  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$50,000 in equipment donation  
Period: NA

Supporting Agency: US Army CRDEC  
Project Title: Chemical Biological Mass Spectrometer / Data Analysis  
Principal Investigator: Peter B. Harrington  
Amount Funded \$25,000 (total costs)  
Period: September 1, 1992 to March 31, 1993.

Supporting Agency: Dow Chemical Company  
Project Title: Prediction of Polymer Properties by Pattern Recognition/Spectroscopic  
Probes  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$5,000 (direct costs)  
Period: NA

Supporting Agency: US Army CRDEC  
Project Title: Chemical Biological Mass Spectrometer / Data Analysis

Principal Investigator: Peter B. Harrington  
Amount Funded \$25,000 (total costs)  
Period: June 6, 1991 to December 20, 1991

Supporting Agency: Charles Evans & Associates  
Project Title: Time of Flight Static Secondary Ion Mass Spectrometry / Pattern Recognition

Principal Investigator: Peter B. Harrington  
Amount Funded: \$11,000 (total costs)  
Period: March 25, 1991 to September 6, 1991

Supporting Agency: Teledyne CME  
Project Title: Chemical Biological Mass Spectrometer  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$65,000 (total costs)  
Period: January 1, 1989 to September 6, 1990

Supporting Agency: Pyrotek  
Project Title: Pyrolysis-Gas Chromatography / Sequence Comparison.  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$10,000 in equipment donation  
Period: NA

Supporting Agency: Nabisco Brands Inc.  
Project Title: Preliminary Investigation of Vegetable Oil Evaluation  
Principal Investigator: Peter B. Harrington  
Amount Funded: \$5,500 (total costs)  
Period Duration: March 1, 1990 to July 1, 1990

### **Patents**

- 1) P.B. Harrington and H.P. Whittenburg, Splitless Pyrolysis Gas Chromatography Injector, U.S. Patent 5,472,670, Dec. 5, 1995.

### **Publications in Progress** (\*Denotes corresponding author, order submitted)

- 1) J. Du, R. Yang\*, H. Mao, J. Li, L. Qu\*, P.B. Harrington, Electrostatic repulsion strategy for highly selective and sensitive "switch -on" fluorescence sensor of ascorbic acid based on the cysteamine-coated CdTe quantum dots and cerium(IV) submitted to *Talanta*.
- 2) P.B. Harrington, Multiple Versus Single Set Validation submitted to *CRC Critical Review in Analytical Chemistry*.
- 3) X. Wang, P.B. Harrington\*, and S.F. Baugh, Comparative Study of NMR Spectral Profiling for the Characterization and Authentication of *Cannabis* in Press at the *Journal of AOAC-Int*.

- 4) X. Zhao and P.B. Harrington\*, Determination of 1,8 Cineole in Fresh Rosemary and Sage Leaves by Solid-phase Microextraction and Gas Chromatography/Mass Spectrometry in press at *Research Analytica*.
- 5) Z. Zhang\*, J. Wang, Y. Liao, Z. Zhang, Y. Xiang, P.B. Harrington, Non-destructive identification of rhubarb samples by terahertz time domain spectroscopy and chemometrics methods submitted to the *Microchemical Journal*.
- 6) Y. Zhou, R. Yang\*, Y.P. Pu, J. Li, L. Qu\*, P.B. Harrington, A ultrasensitive spectrophotometry sensor for tartrazine detection based on poly (diallyldimethylammonium chloride) modified nano-silver submitted to *Sensors & Actuators: B. Chemical*.
- 7) M. Jie, F. Yu, S. Yu, L. Qu, P.B. Harrington, and Y. Wu\*, Study on Magnetic Enzyme Chemiluminescence Immunoassay Methods of Fumonisin B1 submitted to *Biosensors and Bioelectronics*.

**Publications from OU Projects** (\*Denotes corresponding author)

- 1) A.K. Aloglu, P.B. Harrington\*, S. Sahin, C. Demir, and M.E. Gunes, Chemical Profiling of Floral and Chestnut Honey using High-Performance Liquid Chromatography-Ultraviolet Detection, *Journal of Food Composition and Analysis* (2017) **62** 205-210 DOI: 10.1016/j.jfca.2017.06.002.
- 2) Y. Mao, L. Yu\*, R. Yang, C. Ma, L. Qu\*, P.B. Harrington, New peptide inhibitors modulate the self-assembly of islet amyloid polypeptide residues 11-20, *European Journal of Pharmacology* (2017) **804** 102-110 DOI: 10.1016/j.ejphar.2017.03.015.
- 3) P.B. Harrington\* and X. Wang, Spectral Representation of Proton NMR Spectroscopy for the Pattern Recognition of Complex Materials, *Journal of Analysis and Testing* (2017) **1:10** DOI: 10.1007/s41664-017-0003-y.
- 4) P.B. Harrington\*, Automated Support Vector Regression, *Journal of Chemometrics* (2017) **31** 1-14 DOI: 10.1002/cem.2867.
- 5) P.B. Harrington\*, Support Vector Machine Classification Trees Based on Fuzzy Entropy of Classification, *Analytica Chimica Acta* (2017) **954** 14-21 DOI: 10.1016/j.aca.2016.11.072.
- 6) A.K. Aloglu, P.B. Harrington\*, S. Sahin, C. Demir, Prediction of Total Antioxidant Activity of *Prunella* L. Species by Automatic Partial Least Square Regression Applied to 2-Way Liquid Chromatographic UV Spectral Images. *Talanta* (2016) **161** 503-510 DOI: 10.1016/j.talanta.2016.09.014.

- 7) N.R. Saichek, C.R. Cox, S. Kim, P.B. Harrington, N.R. Stambach, and K. Voorhees\*, Strain-level *Staphylococcus* differentiation by CeO<sub>2</sub>-metal oxide laser ionization mass spectrometry fatty acid profiling. *BMC Microbiology* (2016) **16:72** 1-11 DOI: 10.1186/s12866-016-0658-y.
- 8) Z. Chen, Z. Zhang\*, R. Zhu, Y. Xiang, and P.B. Harrington, Diagnosis of patients with chronic kidney disease by using two fuzzy classifiers. *Chemometrics and Intelligent Laboratory Systems* (2016) **153** 140-145 DOI: 10.1016/j.chemolab.2016.03.004.
- 9) J. Li, J. Qu, L. Qu, R. Yang\*, P.B. Harrington, A sensitive electrochemical sensor of quercetin based on graphene quantum dots/gold nanoparticles nanocomposite. *Electrochimica Acta* (2016) **28:6** 1322-1330 DOI: 10.1002/elan.201500490.
- 10) J.M. Harnly\*, P. Chen, J. Sun, H. Huang, K. Colson, J. Yuk, J.A. McCoy, D.H. Reynaud, and P.B. Harrington, MS, NMR, and DNA Barcoding, Complementary Methods for Identification and Authentication of Black Cohosh (*Actaea racemosa* L.). *Planta Medica* (2015) **82:03** 250-262 DOI: 10.1055/s-0035-1558113.
- 11) Y. Mao, L. Yu, R. Yang, C. Ma, L. Qu, and P.B. Harrington, New insights into side effect of solvents on the aggregation of human islet amyloid polypeptide 11–20. *Talanta* (2015) **148** 380-386 DOI: 10.1016/j.talanta.2015.11.012.
- 12) P.B. Harrington\*, Support Vector Machine Classification Trees. *Analytical Chemistry* (2015) **87:21** 11065-11071 DOI: 10.1021/acs.analchem.5b03113.
- 13) J. Harnly\*, P. Chen, K. Colson, J.A. McCoy, D.H. Reynaud, and P.B. Harrington, MS, NMR, and DNA barcoding, complementary methods for identification and authentication of Black Cohosh (*Actaea racemosa* L.). *Planta Medica* (2015) **81:11** PA1 DOI: 10.1055/s-0035-1556184.
- 14) R. Yang\*, D. Miao, Y. Liang, L. Qu, J. Li, P.B. Harrington, Ultrasensitive electrochemical sensor based on CdTe quantum dots-decorated poly(diallyldimethylammonium chloride)-functionalized graphene nanocomposite modified glassy carbon electrode for the determination of puerarin in biological samples. *Electrochimica Acta* (2015) **173:10** 839-846 DOI: 10.1016/j.electacta.2015.05.139.
- 15) Z. Zhang\*, Z. Chen, R. Zhu, Y. Xiang, Y. Yang, and P.B. Harrington, Application of Terahertz Time-Domain Spectroscopy Combined with Chemometrics to Quantitative Analysis of Imidacloprid in Rice Samples.

- Journal of Quantitative Spectroscopy and Radiative Transfer* (2015) **167** 1-9  
DOI: 10.1016/j.jqsrt.2015.07.018.
- 16) A.H. Bani Rashaid, P.B. Harrington\*, and Glen P. Jackson Profiling Amino Acids of Jordanian Scalp Hair as a Tool for Diabetes Mellitus Diagnosis. *Analytical Chemistry* (2015) DOI: 10.1021/acs.analchem.5b00460.
  - 17) M. Zhang, Y. Zhao, P.B. Harrington, and Pei Chen\*, Differentiation of *Aurantii Fructus Immaturus* and *Fructus Ponociri Trifoliatae Immaturus* by Flow-injection with Ultraviolet Spectroscopic Detection and Proton Nuclear Magnetic Resonance using Partial Least-squares Discriminant Analysis. *Analytical Letters* (2015) 10.1080/00032719.2015.1045588.
  - 18) M. Zhang, P.B. Harrington, and P. Chen\*, Classification of Cultivation Locations of Black Pepper (*Piper nigrum* L.) using Gas Chromatography and Chemometrics. *Current Chromatography* (2015) **2** 1-1 DOI: 10.2174/2213240602666150518235059.
  - 19) L. Wang, R. Yang\*, J. Li, L. Qu, and P.B. Harrington, High-sensitive electrochemical sensor of Sudan I based on template-directed self-assembly of graphene-ZnSe quantum dots hybrid structure. *Sensors and Actuators B-Chemical* (2015) **215** 181-187 DOI: 10.1016/j.snb.2015.03.034.
  - 20) M. Zhang and P.B. Harrington\*, Application of Chemometrics to Resolve Overlapping Mass Spectral Peak Clusters Between Trichloroethylene and its Deuterated Internal Standard. *Rapid Communications in Mass Spectrometry* (2015) **29** 789-794 DOI: 10.1002/rcm.7164.
  - 21) G. Downey, L.L. Botros\*, J. Jablonski, C. Chang, M.M. Bergana, P. Wehling, J.M. Harnly, P.B. Harrington, A.R. Potts, and J.C. Moore, Exploring the variance of authentic skim and non-fat dry milk powder spectra. *NIR News* (2015) **26:2** 11-14 DOI: 10.1255/nirn.1512.
  - 22) M. Zhang and P.B. Harrington\*, Determination of Trichloroethylene in Water by Liquid-Liquid Microextraction Assisted Solid Phase Microextraction. *Chromatography* (2015) **2:1** 66-78 DOI: 10.3390/chromatography2010066.
  - 23) L. Wang, R. Yang\*, H. Wang, J. Li, L. Qu\*, and P.B. Harrington, High-selective and sensitive voltammetric sensor for butylated hydroxyanisole based on AuNPs-PVP-graphene nanocomposites. *Talanta* **138:1** (2015) 169-175 DOI: 10.1016/j.talanta.2015.01.016.
  - 24) Y. Mao, L. Yu\*, J. Li, L. Qu\*, and P.B. Harrington, A novel method for the study of molecular interaction by using microscale thermophoresis. *Talanta* **132** (2015) 894-901 DOI: 10.1016/j.talanta.2014.09.038.

- 25) N. Qi, Z. Zhang\*, Y. Xiang, Y. Yang, X. Liang, and P.B. Harrington, Terahertz time-domain spectroscopy combined with support vector machines and partial least squares-discriminant analysis applied for the diagnosis of cervical carcinoma. *Analytical Methods* **7:6** (2015) 2333-2338 DOI: 10.1039/C4AY02665A.
- 26) A.H. Bani Rashaid, P.B. Harrington, and G.P. Jackson\*, Amino Acid Composition of Human Scalp Hair as a Biometric Classifier and Investigative Lead. *Analytical Methods* **7:5** (2015) 1707-1718 DOI: 10.1039/C4AY02588A.
- 27) N. Qi, Z. Zhang\*, Y. Xiang, Y. Yang, and P.B. Harrington, Terahertz Time-domain Spectroscopy Combined with Fuzzy Rule-building Expert System and Fuzzy Optimal Associative Memory Applied to Early Diagnosis of Cervical Carcinoma. *Medical Oncology* **32:1** (2014) 1-6 DOI: 10.1007/s12032-014-0383-z.
- 28) K.J. Voorhees\*, N.R. Saichek, K.R. Jensen, C.R. Cox, and P.B. Harrington, Comparison of Metal Oxide Catalysts for Pyrolytic MALDI-TOF MS Bacterial Identification. *Journal of Analytical and Applied Pyrolysis* (2014) DOI: 10.1016/j.jaap.2014.10.016.
- 29) Z. Wang, L. Lin, J.M. Harnly, P.B. Harrington, and P. Chen\*, Computer-aided method for identification of major flavone/flavonol glycosides by high-performance liquid chromatography-diode array detection-tandem mass spectrometry (HPLC-DAD-MS/MS). *Analytical and Bioanalytical Chemistry* **406** (2014) 7695-7704 DOI: 10.1007/s00216-014-8187-8.
- 30) D. Miao, J. Li, R. Yang\*, J. Qu, L. Qu, and P.B. Harrington, Supersensitive electrochemical sensor for the fast determination of rutin in pharmaceuticals and biological samples based on poly(diallyldimethylammonium chloride)-functionalized graphene. *Journal of Electroanalytical Chemistry* **732** (2014) 17-24 DOI: 10.1016/j.jelechem.2014.08.018.
- 31) M. Zhang and P.B. Harrington\*, Simultaneous Quantification of Aroclor Mixtures in Soil Samples by Gas Chromatography/Mass Spectrometry with Solid Phase Microextraction using Partial Least-Squares Regression. *Chemosphere* **118C** (2014) 187-193, DOI: 10.1016/j.chemosphere.2014.08.018.
- 32) Z. Wang, M. Zhang, and P.B. Harrington\*, A Comparison of Three Algorithms for the Baseline Correction of Hyphenated Data Objects. *Analytical Chemistry* **86:18** (2014) 9050-9057, DOI: 10.1021/ac501658k.
- 33) L. Wang, R. Yang\*, J. Chen, J. Li, L. Qu\*, and P.B. Harrington, Sensitive



- voltammetric sensor based on Isopropanol–Nafion–PSS–GR nanocomposite modified glassy carbon electrode for determination of Clenbuterol in pork. *Food Chemistry* **164** (2014) 113-118, DOI: 10.1016/j.foodchem.2014.04.052.
- 34) A.H. Bani Rashaid, G.P. Jackson, and, P.B. Harrington\*, Validation of a Method of Measuring the Amino Acid Composition of Proteins by Gas Chromatography/Mass Spectrometry. *Enliven: Bio Analytical Techniques* **1:002** (2014), <http://www.enlivenarchive.org/bioanalytical-002.pdf>.
- 35) M. Zhang, G.P. Jackson, N.A. Kruse, J.R. Bowman, and P.B. Harrington\*, Determination of Aroclor 1260 in Soil Samples by GC-MS with Solid-Phase Microextraction. *Journal of Separation Science* **118** (2014) 187-193, DOI: 10.1002/jssc.201400102.
- 36) J.M. Harnly\*, P.B. Harrington\*, L.L. Botros, J.E. Jablonski, C. Chang, M.M. Bergana, P. Wehling , G. Downey, A.R. Potts , and J.C. Moore, Characterization of Near Infrared Spectral Variance in the Authentication of Skim and Nonfat Dry Milk Powder Collection Using ANOVA-PCA, Pooled-ANOVA, and Partial Least Squares Regression. *Journal of Agriculture and Food Chemistry* **62:32** (2014) 8060-8067, DOI: 10.1021/jf5013727.
- 37) J. Wang, Z. Zhang\*, Z. Zhang, Y. Xiang, and P.B. Harrington, THz-TDS combined with a fuzzy rule-building expert system applied to identification of official rhubarb samples. *Analytical Methods* **6:19** (2014) 7695-7702, DOI: 10.1039/C4AY00555D.
- 38) P.B. Harrington\*, Fuzzy Grid Encoded Independent Modeling for Class Analogies (FIMCA). *Analytical Chemistry* **86:10** (2014) 4883-4892, DOI: 10.1021/ac5001543.
- 39) J. Li, D. Miao, R. Yang, L. Qu, and P.B. Harrington, Synthesis of poly(sodium 4-styrenesulfonate) functionalized graphene/cetyltrimethylammonium bromide (CTAB) nanocomposite and its application in electrochemical oxidation of 2,4-dichlorophenol. *Electrochimica Acta* **125** (2014) 1-8.
- 40) F. Yu, S. Yu, L. Yu, Y. Li, Y. Wu\*, H. Zhang, L. Qu, P.B. Harrington, Determination of residual enrofloxacin in food samples by a sensitive method of chemiluminescence enzyme immunoassay. *Food Chemistry* **149** (2014) 71-75 DOI: 10.1016 /j.foodchem.2013.10.024.
- 41) J.M. Harnly\*, P. Chen, and P.B. Harrington, Probability of Identification: Adulteration of American Ginseng with Asian Ginseng. *Journal of AOAC International* **96** (2013) 1258-1265 DOI: 10.5740/jaoacint.13-290.

- 42) M. Zhang and P.B. Harrington\*, Automated Pipeline for Classifying Aroclors in Soil by Gas Chromatography/Mass Spectrometry using Modulo Compressed Two-way Data Objects, *Talanta* **117** (2013) 483-491 DOI: 10.1016/j.talanta.2013.09.050.
- 43) H. Zhang, Y. Wu\*, F. Yu, S. Yu, H. Zhang, L. Qu, P.B. Harrington, Study on the reaction mechanism and the static injection chemiluminescence method for detection of acetaminophen, *Luminescence* **28:6** (2013) 905-909 DOI: 10.1002/bio.2455.
- 44) Z. Wang and P.B. Harrington\*, Feature Selection from Gas Chromatography/Mass Spectrometry Data Using a Bootstrapped Fuzzy Rule-Building Expert System, *Analytical and Bioanalytical Chemistry* **405** (2013) 9219-9234, DOI: 10.1007/s00216-013-7327-x.
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- 47) G. Wang, M. Ma, Z. Zhang\*, Y. Xiang, and P.B. Harrington, A novel DPSO-SVM system for variable interval selection of endometrial tissue sections by near infrared spectroscopy. *Talanta* **112** (2013) 136-142, DOI: 10.1016/j.talanta.2013.03.016.
- 48) Z. Wang, P. Chen, L. Yu, and P.B. Harrington\*, Authentication of Organically and Conventionally Grown Basil by Gas Chromatography/Mass Spectrometry Chemical Profiles. *Analytical Chemistry* **85:5** (2013) 2945-2953, DOI: 10.1021/ac303445v.
- 49) N. Qi, Z. Zhang\*, Y. Xiang, and P.B. Harrington, Locally linear embedding method for dimensionality reduction of tissue sections of endometrial carcinoma by near infrared spectroscopy. *Analytica Chimica Acta* **724** (2012) 12-19.
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*Biomolecular Spectroscopy* **93** (2012) 164-168.

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- 52) Z. Wang, Y. Zhang, H. Zhang, P.B. Harrington\*, H. Chen\*, Fast and Selective Modification of Thiol Proteins/Peptides by N-(Phenylseleno) phthalimide, *Journal of the American Society for Mass Spectrometry* **23:3** (2012) 520-529 DOI: 10.1007/s13361-011-0317-3.
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- 62) X. Sun, C.M. Zimmermann, G.P. Jackson, C.E. Bunker, and P.B. Harrington\*, Classification of Jet Fuels by Fuzzy Rule-Building Expert Systems Applied to Two-Way Data by Fast Gas Chromatography-Fast Scanning Quadrupole Ion Trap Mass Spectrometry. *Talanta*, **83:4** (2011) 1260-1268.
- 63) Z. Xu, C.E. Bunker, and P.B. Harrington\*, Classification of Jet Fuel Properties by Near Infrared Spectroscopy Using Fuzzy Rule-Building Expert Systems and Support Vector Machines. *Applied Spectroscopy*, **64:11** (2010) 1251-1258.
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- 15) E.S. Reese, J.Y. Tong, P.B. Harrington\*, and D.M. Davis, Interactive Self-Modeling Analysis of Ion Mobility Spectra. The Conference Proceedings of the Fifth International Workshop on Ion Mobility Spectrometry, August, 1996, 275-292.
- 16) P.B. Harrington\*, P. Zheng, and D.M. Davis, Quantitative Analysis of Ion Mobility Spectra Using Automated Fourier Self-Deconvolution and Temperature Constrained Cascade Correlation Neural Network. The Conference Proceedings of the Fourth International Workshop on Ion Mobility Spectrometry, August, 1995, 1-12.
- 17) P.B. Harrington, Temperature Constrained-Cascade Correlation Networks.

Proceedings of the Adaptive Parallel Computing Symposium-96, Dayton, OH, August 8-9, 1996, 155-164.

- 18) P.B. Harrington\*, P. Zheng and D.M. Davis, Quantitative Analysis of Volatile Organic Compounds Using Ion Mobility Spectra and Neural Networks. The NASA Conference Proceedings of the Third International Workshop on Ion Mobility Spectrometry, Publication #3301, October, 1994, 312-333.
- 19) P.B. Harrington, Fuzzy Rule-Building Expert Systems. *Computer Enhanced Analytical Spectroscopy*, III, ed P.C. Jurs, Plenum Press: New York, NY, 1992, 239-258.
- 20) K.J. Voorhees\*, P.B. Harrington, T.E. Street, S. Hoffman, S.L. Durfee, J.E. Bonelli and C.S. Firnhaber, Approaches to Pyrolysis Mass Spectrometry Data Analysis of Biological Materials. *Computer Enhanced Analytical Spectroscopy*, II, ed. H.L.C. Meuzelaar, New York: Plenum Publishing Corp. 1989.

#### **Book and Software Reviews**

- 1) P. B. Harrington, Review of Differential Ion Mobility Spectrometry: Nonlinear Ion Transport and Fundamentals of FAIMS by Alexandre A. Shvartsburg, *Journal of the American Chemical Society*, **132:20** (2010) 7230.
- 2) P.B. Harrington review of Nature Inspired Methods in Chemometrics: Genetic Algorithms and Artificial Neural Networks, edited by Riccardo Leardi, *Applied Spectroscopy*, **59:4** (2005) 94A.
- 3) P.B. Harrington review of Design and Analysis in Chemical Research edited by Roy L. Tranter, *The Analyst*, <http://www.rsc.org/is/journals/current/analyst/anlrev07.htm>, date accessed 24-Aug-2001.
- 4) P.B. Harrington, review of Pirouette: a chemometrics toolbox. *Analytical Chemistry*, **69** (1997) 248A-249A.
- 5) P.B. Harrington, review of Bioinformatics: From Nucleic Acids to Cell Metabolism. *Chemometrics and Intelligent Laboratory Systems*, **35** (1996) 137.
- 6) P.B. Harrington, review of Mathematical Modeling in Chemistry. *Vibrational Spectroscopy*, **4:2** (1993) 262.
- 7) P.B. Harrington, Review of Computational Chemistry Using the P.C. *Vibrational Spectroscopy*, **1** (1991) 401.
- 8) P.B. Harrington, review of Microcomputers and Laboratory Instrumentation, 2nd Edition. *Analytical Chemistry*, **61** (1989) 856A.



## **Presentations**

### **Mentoring**

- 1) P.B. Harrington, "The Art of Writing Scientific Research Papers", Zhengzhou University, Zhengzhou, PRC, May 25, 2016.
- 2) P.B. Harrington, "Introduction to Chemometrics", The Colorado School of Mines, Golden, CO, November 8, 2010.
- 3) P.B. Harrington, "Chemistry Opportunities at OHIO University", Beijing Institute of Technology, Beijing, PRC, July 1, 2008.
- 4) P.B. Harrington, "Analytical and Forensic Chemistry at Ohio University", Shanghai Jiao Tong University, Shanghai, PRC, December 16, 2006.
- 5) P.B. Harrington, "Department of Chemistry and Biochemistry at Ohio University", Shanghai Jiao Tong University, Shanghai, PRC, December 16, 2006.
- 6) P.B. Harrington, "Analytical and Forensic Chemistry at Ohio University", Tongji University, Shanghai, PRC, December 16, 2006.
- 7) P.B. Harrington, "Department of Chemistry and Biochemistry at Ohio University", Tongji University, Shanghai, PRC, December 16, 2006.
- 8) P.B. Harrington, "Analytical and Forensic Chemistry at Ohio University", Shanghai University, Shanghai, PRC, December 13, 2006.
- 9) P.B. Harrington, "Department of Chemistry and Biochemistry at Ohio University", Shanghai University, Shanghai, PRC, December 13, 2006.
- 10) P.B. Harrington, "Introduction to Chemometrics: The Multivariate Perspective" lecture (1.5 hr) given to an undergraduate class at Universität Leipzig, Leipzig, Germany, July 14, 2004.
- 11) P.B. Harrington, "Experimental Design and Optimization" lecture (1.5 hr) given to an undergraduate class at Universität Leipzig, Leipzig, Germany, July 15, 2004.
- 12) P.B. Harrington, "Ohio University's Graduate Program in Chemistry" presented at the Second Ohio Analytical Chemistry Consortium, Columbus, OH, October 31, 2003.
- 13) P.B. Harrington, "Statistical Experimental Design for Chemists" presented at Ohio University, Athens, OH, April 28, 2003.
- 14) P.B. Harrington, "Ohio University's Graduate Program in Chemistry"

presented at the First Ohio Analytical Chemistry Consortium, Columbus, OH, November 8, 2002.

### **Invited Scientific Presentations at Universities and Colleges**

- 1) P.B. Harrington, "Bootstrapping as a Tool to Automate Chemometric Methods", Capital Normal University, Beijing, China, May 10, 2017.
- 2) P.B. Harrington, "Chemometric Tools for the Characterization of Complex Materials", Tsinghua University, Beijing, China, May 9, 2017.
- 3) P.B. Harrington, "Chemometric Tools for the Characterization of Complex Materials", University of Science and Technology Beijing, Beijing, China, May 8, 2017.
- 4) P.B. Harrington, "Bootstrapping as a Tool to Automate and Validate Chemometric Methods", Kwansai Gakuin University, Shin Sanda, Japan, March 21, 2017.
- 5) P.B. Harrington, "Application of Support Vector Machine Classification Trees to the Authentication of Traditional Chinese Medicines", Zhengzhou University, Zhengzhou, PRC, May 25, 2016.
- 6) P.B. Harrington, "Application of Support Vector Machine Classification Trees to the Authentication of Traditional Chinese Medicines", Hunan University of Traditional Medicine, Changsha, PRC, May 24, 2016.
- 7) P.B. Harrington, "Application of Support Vector Machine Classification Trees to the Authentication of Traditional Chinese Medicines", Capital Normal University, Beijing, PRC, May 7, 2016.
- 8) P.B. Harrington, "Application of Support Vector Machines to Chemometrics and the Authentication of Complex Materials", Department of Chemistry and Geochemistry, Colorado School of Mines, Golden, CO, January 15, 2016.
- 9) P.B. Harrington, "Novel Multiclass Support Vector Machine Classification Tree Algorithm and its Application to Authentication of Traditional Chinese Medicines", College of Chemistry, Wuhan University, Wuhan, PRC, July 1, 2015.
- 10) P.B. Harrington, "Chemometric Opportunities for Forensic Chemical Analysis", Department of Photochemistry, Bowling Green State University, Bowling Green, OH, December 8, 2014.
- 11) P.B. Harrington, "Fuzzy Optimal Associative Memories for Modeling Chemical Profiles: Authentication of Foods and Nutraceuticals", College of Pharmacy,

Wuhan University, Wuhan, PRC, November 26, 2013.

- 12) P.B. Harrington, "Fuzzy Optimal Associative Memories for Modeling Chemical Profiles: Authentication of Foods and Nutraceuticals", College of Chemistry, Wuhan University, Wuhan, PRC, November 25, 2013.
- 13) P.B. Harrington, "Fuzzy Optimal Associative Memories for Modeling Chemical Profiles: Authentication of Foods and Nutraceuticals", Capital Normal University, Beijing, PRC, November 18, 2013.
- 14) P.B. Harrington, "Fuzzy Optimal Associative Memories for the Authentication of Nutraceuticals by Mass Spectrometry", Shanghai University, Shanghai, PRC, October 15, 2012.
- 15) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Capital Normal University, Beijing, PRC, March 21, 2012.
- 16) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Wuhan University, Wuhan, PRC, November 29, 2011.
- 17) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Renmin University, Beijing, PRC, August 2, 2011.
- 18) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Tsinghua University, Beijing, PRC, July 28, 2011.
- 19) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Zhengzhou University, Zhengzhou, PRC, July 25, 2011.
- 20) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Henan University, Kaifeng, PRC, July 19, 2011.
- 21) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Beijing Normal University, Beijing Normal University, PRC, March 18, 2011.
- 22) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Capital Normal University, Beijing, PRC, March 17, 2011.
- 23) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Chinese Peoples Public Security University, Beijing, PRC, December 16, 2010.
- 24) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Shanghai University, Shanghai, PRC, December 9, 2010.

- 25) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Yangzhou University, Yangzhou, PRC, December 6, 2010.
- 26) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", The Colorado School of Mines, Golden, CO, November 9, 2010.
- 27) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Universitetet i Bergen, Bergen, NO, August 31, 2010.
- 28) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Guizhou Normal University, Guiyang, PRC, July 23, 2010.
- 29) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Capital Normal University, Beijing, PRC, July 21, 2010.
- 30) P.B. Harrington, "Three -ics : Chemometrics, Forensics, and Proteomics", Shenyang Medical University, College of Forensic Science, Shenyang, PRC, December 16, 2009.
- 31) P.B. Harrington, "Three -ics : Chemometrics, Forensics, and Proteomics", Shanghai Institute of Organic Chemistry, Shanghai, PRC, December 14, 2009.
- 32) P.B. Harrington, "Three -ics : Chemometrics, Forensics, and Proteomics", Shanghai University, Shanghai, PRC, December 12, 2009.
- 33) P.B. Harrington, "Three -ics : Chemometrics, Forensics, and Proteomics", Capital Normal University, Beijing, PRC, December 10, 2009.
- 34) P.B. Harrington, "Three -ics : Chemometrics, Forensics, and Proteomics", Shandong Normal University, Jinan, PRC, August 21, 2009.
- 35) P.B. Harrington, "Chemometric Opportunities in Forensic Chemical Analysis", Shanghai University, Shanghai, PRC, April 3, 2009.
- 36) P.B. Harrington, "Chemometric Opportunities in Forensic Chemical Analysis", University of Central China, Changsha, PRC, March 30, 2009.
- 37) P.B. Harrington, "Chemometric Opportunities in Forensic Chemical Analysis", Capital Normal University, Beijing, PRC, March 26, 2009.
- 38) P.B. Harrington, "Introduction to Forensic Chemical Analysis", Capital Normal University, Beijing, PRC, March 24, 2009. (Undergraduate Lecture)

- 39) P.B. Harrington, "Chemometric Opportunities in Forensic Chemical Analysis", Paul Cézanne Université, Marseille, France, December 12, 2008.
- 40) P.B. Harrington, "Three -ics: Chemometrics, Forensics, and Proteomics", Universitat Rovira I Virgili, Tarragona, Spain, November 12, 2008.
- 41) P.B. Harrington, "Three -ics: Chemometrics, Forensics, and Proteomics", Agder University College, Kristiansand, Norway, November 6, 2008.
- 42) P.B. Harrington, "Two Factor ANOVA-PCA of NIR Spectra from Olive Oils", Paul Cézanne Université, Marseille, France, October 2, 2008.
- 43) P.B. Harrington, "Chemometric Opportunities in the Discovery of Proteomic Biomarkers via Mass Spectrometry", Peking University, Beijing, PRC, July 4, 2008.
- 44) P.B. Harrington, "Three -ics: Chemometrics, Forensics, and Proteomics", Beijing Institute of Technology, Beijing, PRC, July 1, 2008.
- 45) P.B. Harrington, "Enhanced Detection of Explosives by Ion Mobility Spectrometry and Chemometrics", Beijing General Research Institute of Mining and Metallurgy, Beijing, PRC, December 6, 2007.
- 46) P.B. Harrington, "Enhanced Detection of Explosives by Ion Mobility Spectrometry and Chemometrics", Capital Normal University, Beijing, PRC, December 4, 2007.
- 47) P.B. Harrington, "Three -ics: Chemometrics, Forensics, and Proteomics", University of Missouri, Columbia, MO, October 19, 2007.
- 48) P.B. Harrington, "Chemometric Opportunities in the Discovery of Proteomic Biomarkers via Mass Spectrometry", Zhongshan University, Guangzhou, PRC, September 28, 2007.
- 49) P.B. Harrington, "Chemometric Opportunities in the Discovery of Proteomic Biomarkers via Mass Spectrometry", Shanghai University, Shanghai, PRC, September 21, 2007.
- 50) P.B. Harrington, Yao Lu, and Ping Chen, "Ion and Differential Mobility Spectrometries: Portable Tools for Forensic Investigations", Capital Normal University, Beijing, PRC, March 22, 2007.
- 51) P.B. Harrington, "Bootstrap Methods in MALDI-MS: How to Get Something from Nothing", Tongji University, Shanghai, PRC, December 15, 2006.
- 52) P.B. Harrington, "Bootstrap Methods in MALDI-MS: How to Get Something

- from Nothing", Shanghai University, Shanghai, PRC, December 11, 2006.
- 53) P.B. Harrington, Yao Lu, and Ping Chen, "Classification Of Two-way Data for Forensic Fingerprinting of Fuels by Chromatography-Mass Spectrometry and Gas Chromatography-Differential Mobility Spectrometry", North East Normal University, Changchun, PRC, December 7, 2006.
  - 54) P.B. Harrington, "Bootstrap Methods in MALDI-MS: How to Get Something from Nothing", Capital Normal University, Beijing, PRC, December 6, 2006.
  - 55) P.B. Harrington, Y. Lu, P. Chen, J.J. Karnes, and C.E. Bunker, "Classification Of Two-way Data for Forensic Fingerprinting of Fuels by Chromatography-Mass Spectrometry and Gas Chromatography-Differential Mobility Spectrometry", Department of Chemistry & Biochemistry, Ohio University, Athens, OH, October 5, 2006.
  - 56) P.B. Harrington, Ping Chen, Preshious Rearden, and Yao Lu, "Chemometric Opportunities in Forensic Chemical Analysis", The Richard Stockton College of New Jersey, Atlantic City, NJ, December 7, 2005.
  - 57) P.B. Harrington, Ping Chen, Preshious Rearden, and Yao Lu, "Forensic Adventures with Ion Mobility Spectrometry and Chemometrics", University of West Virginia, Morgantown, WV, September 28, 2005.
  - 58) P.B. Harrington, Ping Chen, and Mariela Ochoa, "Chemometric Tools for Mass Spectrometry of the Proteome", Applied and Computational Mathematics Seminar, Ohio University, Athens, OH, February 8, 2005.
  - 59) P.B. Harrington, "Chemometric Modeling of Ion Mobility and Mass Spectrometric Data", presented at East Carolina University, Greenville, NC, December 3, 2004.
  - 60) P.B. Harrington, M.L. Ochoa, N.E. Vieira, C. Laurent, S.P. Markey, and A.L. Yergey, "Chemometric Considerations in Proteomic Analyses by Mass Spectrometry", presented at Shanghai University, Shanghai, China, October 21, 2004.
  - 61) A.L. Yergey, P.B. Harrington, N.E. Vieira, and R. Romero, "Mass Spectrometric Profiling for Disease Diagnosis: Development of Methodology" presented at the University of Calgary Faculty of Medicine, Calgary, CA, September 30, 2004.
  - 62) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility Spectrometries" presented at Universität Leipzig, Leipzig, Germany, July 15, 2004.

- 63) P.B. Harrington, "Forensic Adventures with Ion Mobility and Mass Spectrometries" presented at Ohio Wesleyan University, Delaware, OH, March 19, 2004.
- 64) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at Universitat Rovira I Virgili, Tarragona, Spain, July 24, 2003.
- 65) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at University of Barcelona, Barcelona, Spain, July 22, 2003.
- 66) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at San Jose State University, San Jose, CA, May 13, 2003.
- 67) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at University of New Mexico, Albuquerque, NM, May 2, 2003.
- 68) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at New Mexico State University, Las Cruces, NM, May 1, 2003.
- 69) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at New Mexico Institute of Mining and Technology, Socorro, NM, April 30, 2003.
- 70) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at University of Wisconsin Stevens Point, Stevens Point, WI, April 11, 2003.
- 71) P.B. Harrington, T. Buxton, and G. Chen, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at Indiana University of Pennsylvania, Indiana, PA, December 6, 2002.
- 72) P.B. Harrington, T. Buxton, and G. Chen, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at the Idaho State University, Pocatello, ID, February 8, 2002.
- 73) P.B. Harrington, T. Buxton, and G. Chen, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at Montana State University, Bozeman, MT, November 16, 2001.
- 74) P.B. Harrington, T. Buxton, G. Chen, A. Urbas, L. Shaw, and A. Mehay, "Chemometrics: New Tools for Solving Old Problems" presented at the

University of Wisconsin, Milwaukee, Milwaukee, WI, May 7, 2001.

- 75) P.B. Harrington, T. Buxton, G. Chen, A. Urbas, L. Shaw, and A. Mehay, "Chemometrics: New Tools for Solving Old Problems" presented at the University of Central Arkansas, Conway, AR, April 20, 2001.
- 76) P.B. Harrington, T. Buxton, G. Chen, A. Urbas, L. Shaw, and A. Mehay, "Chemometrics: New Tools for Solving Old Problems" presented at Fairleigh Dickinson University, Madison, NJ, April 10, 2001.
- 77) P.B. Harrington, T. Buxton, G. Chen, A. Urbas, L. Shaw, and A. Mehay, "Chemometrics: New Tools for Solving Old Problems" presented at Indiana State University, Terre Haute, IN, April 3, 2001.
- 78) P.B. Harrington, T. Buxton, G. Chen, A. Urbas, L. Shaw, and A. Mehay, "Chemometrics: New Tools for Solving Old Problems" presented at Ohio University, Athens, OH, September 15, 2000.
- 79) P.B. Harrington, C. Cai, J. Wan, T. Buxton, S. Slagel, and L. Shaw, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility Spectrometry" presented at Dalhousie University, Halifax, NS, August 17, 2000.
- 80) P.B. Harrington, C. Cai, J. Wan, S. Slagel, and A. Urbas, "Making the Connection Between Neural Networks and Chemical Sensors" presented at Duquesne University, Pittsburgh, PA, December 3, 1999.
- 81) P.B. Harrington, C. Cai, J. Wan, T. Buxton, S. Slagel, and L. Shaw, "Chemometrics: New Tools for Solving Old Problems" presented at St. Vincent College, Latrobe, PA, March 26, 1999.
- 82) P.B. Harrington, C. Cai, J. Wan, T. Buxton, S. Slagel, and L. Shaw, "Making the Connection Between Neural Networks and Chemical Sensors" presented at La Salle University, Philadelphia, PA, March 25, 1999.
- 83) P.B. Harrington, "Ion Mobility Spectrometry: Detection of pollutants, explosives, and drugs using a handheld instrument" presented at Indiana University of Pennsylvania, Indiana, PA, September, 1998.
- 84) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems" presented at the Virginia Commonwealth University, Richmond, VA, January, 20, 1998.
- 85) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems" presented at University of North Carolina, Chapel Hill, NC, February 10, 1997.



- 86) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems" presented at Northern Arizona University, Flagstaff, AZ, November 15, 1996.
- 87) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems" presented at the Arizona State University Department of Chemistry, Tempe, AZ, November 14, 1996.
- 88) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems" presented at the Clemson University Department of Chemistry, Clemson, SC, September 19, 1996.
- 89) P.B. Harrington, "Making the Connection Between Neural Networks and Analytical Chemistry" presented at De Pauw University, Greencastle, IN, March 14, 1996.
- 90) P.B. Harrington, "Making the Connection Between Neural Networks and Mass Spectrometry" presented at University of Wales, Swansea, United Kingdom, August 18, 1995.
- 91) P.B. Harrington, P. Zheng, P. Tandler, and B. Wabuye, "Making the Connection: Neural Networks and Chemistry" presented at Northern Kentucky University, KY, March 20, 1995.
- 92) P.B. Harrington, "Making the Connection: Neural Networks and Chemistry" presented at John Carrol University, Cleveland, OH, October 26, 1994.
- 93) P.B. Harrington, "Chemometrics: New Approaches to Solving Old Problems" presented at Xavier University, Cincinnati, OH, September 16, 1994.
- 94) P.B. Harrington, "Spectroscopic Uses of Machine Learning: How to Make Computers Take the Initiative" presented at Indiana University of Pennsylvania, Indiana, PA, October 22, 1993.
- 95) P.B. Harrington, "New Directions in Analytical Chemistry" guest lecturer in conjunction with the Randolph-Macon Chemistry Department's lecture series, Ashland, November, 1990.
- 96) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Marshall University, Huntington, WV, March 1990.
- 97) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Kent State University, Kent, OH, February 1989.
- 98) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Seton Hall University, East Orange, NJ, March

1990.

- 99) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Ohio University, Athens, OH, March 1989.
- 100) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Auburn University, Auburn, AL, March 1989.
- 101) P.B. Harrington, "Statistical Tests for Analytical Chemists" presented at Utah State University, Logan, UT, March, 1985.
- 102) P.B. Harrington, "Pyrolysis Gas Chromatography" presented at University of North Carolina, Chapel Hill, NC, March, 1984.
- 103) P.B. Harrington, "Flavor Modeling Using Headspace and Pyrolysis Gas Chromatography," presented at Randolph-Macon College, Ashland, November, 1981.
- 104) P.B. Harrington, "Flavor Chemistry at Standard Brands," presented at Randolph-Macon College, Ashland, November, 1980.

#### **Presentations at Government and Industry**

- 1) P.B. Harrington, "Application of Support Vector Machines to Chemometrics and the Authentication of Complex Materials", Cannaprint, Inc., Broomfield, CO, January 16, 2016.
- 2) P.B. Harrington, "Statistically General Chemometric Models I", IVL Swedish Environmental Research Institute, Stockholm, SE, August 24, 2010.
- 3) P.B. Harrington, "Statistically General Chemometric Models II", IVL Swedish Environmental Research Institute, Stockholm, SE, August 24, 2010.
- 4) P.B. Harrington, "Statistically General Chemometric Models III", IVL Swedish Environmental Research Institute, Stockholm, SE, August 24, 2010.
- 5) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Beltsville Human Nutrition Research Center, USDA/ARS, Beltsville, MD, June 28, 2010.
- 6) P.B. Harrington, "Chemometric Opportunities in Forensic Chemical Analysis", Institute of Forensic Science, Ministry of Justice, Shanghai, PRC, April 2, 2009.
- 7) P.B. Harrington, "Recruiting Undergraduate Baccalaureate Science Majors", EIC, Group, Shanghai, PRC, April 1, 2009 (teleconference with offices in Beijing, Guangzhou, and Nanjing).

- 8) P.B. Harrington, Yao Lu, and Ping Chen, "Ion and Differential Mobility Spectrometries: Portable Tools for Forensic Investigations", National Institutes of Standards and Technology, Gaithersburg, MD, August 30, 2007.
- 9) P.B. Harrington, "Bootstrap Methods in MALDI-MS: How to Get Something from Nothing", National Institutes of Health, Bethesda, MD, November 9, 2006.
- 10) Y. Lu and P.B. Harrington, "Classification of Accelerants from Fire Debris by Gas Chromatography-Differential Mobility Spectrometry (GC-DMS) and Pattern Recognition", National Center of Forensic Science, Orlando, FL, March 14, 2006.
- 11) P.B. Harrington, P. Chen, and M.L. Ochoa, "Chemometric Tools for Mass Spectrometry of the Proteome", US Food and Drug Administration, Center for Food Safety and Applied Nutrition, College Park, MD, August 11, 2005.
- 12) N.E. Vieira, P.B. Harrington, R. Romero, and A.L. Yergey, "Mass Spectral Profiling of Amniotic Fluid", presented at the National Institutes of Health, *Exploring the Proteome III - The Challenge of Cellular Dynamics*, Bethesda, MD, April 15, 2005.
- 13) P. Chen and P.B. Harrington, "Sensor Fusion: Ion Mobility Spectrometry and Infrared Spectroscopy", presented at Edgewood Chemical Biological Center, Edgewood, MD, February 17, 2005.
- 14) P.B. Harrington and P. Chen, "Sensor Fusion: Lightweight Chemical Detector", presented at the Homeland Security Advanced Research Project Agency Kickoff Meeting, Edgewood Chemical Biological Center, Edgewood, MD, February 17, 2005.
- 15) P.B. Harrington, P. Chen, and M.L. Ochoa, "Chemometric Tools for Mass Spectrometry of the Proteome", presented at Battelle, Columbus, OH, February 1, 2005.
- 16) P.B. Harrington, C. Laurent, and S. Markey, "Fuzzy Entropy Classification Systems and Their Application to Mass Spectrometry of the Proteome" presented at the National Institutes of Health/National Institute of Mental Health, Bethesda, MD, December 9, 2004.
- 17) C. Laurent, P. Levitt, D.F. Levinson, P.B. Harrington, S.A. Schwartz, D.B. Campbell, J.L. Norris, P.J. Woods, L. Snider, S. Swedo, H.R. Aerni, R. Moharram, P. Ebert, P. Chaurand, B. Martin, R.M. Caprioli, and S. Markey, "Proteomic studies by MALDI-TOF MS and by SELDI-MS: Methodological Issues" presented at The Intramural Research Program's Scientific Retreat, National Institutes of Health, Bethesda, MD, September 14, 2004.

- 18) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at Bruker Daltonics, Leipzig, Germany, July 16, 2004.
- 19) P. B. Harrington, M.L. Ochoa, S.P. Markey, C. Laurent, K. Saito, & A.L. Yergey, "Chemometric Considerations in Proteomic Analyses by Mass Spectrometry", presented at the National Institutes of Health/National Institute of Child Health and Human Development, Washington DC, May 12, 2004.
- 20) P. B. Harrington, M.L. Ochoa, S.P. Markey, C. Laurent, K. Saito, & A.L. Yergey, "Chemometric Considerations in Proteomic Analyses by Mass Spectrometry", presented at Amgen, Inc., Thousand Oaks, CA, March 26, 2004.
- 21) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at Wright-Patterson Air Force Base, Fuel Research Group," Dayton, OH, May 22, 2003.
- 22) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at Los Alamos National Laboratory, Los Alamos, NM, April 29, 2003.
- 23) P.B. Harrington, "Chemometrics New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at the National Institutes of Health, Washington DC, December 19, 2002.
- 24) P.B. Harrington, T.L. Buxton, and G. Chen, "Strategies for Intelligent Sensors" presented at Wright-Patterson Air Force Base, Fuel Research Group," Dayton, OH, August 28, 2002.
- 25) P.B. Harrington, T.L. Buxton, G. Chen, and N.L. Schmitt, "Chemometrics Opportunities for Ion Mobility Spectrometry" presented at Ion Track Instruments, Wilmington, MA, August 23, 2002.
- 26) P.B. Harrington, T.L. Buxton, G. Chen, and N. Shaw, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility and Mass Spectrometries" presented at the Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID, August 9, 2001.
- 27) P.B. Harrington, T.L. Buxton, G. Chen, and A. Urbas, "Chemometric Strategies for Ion Mobility and Mass Spectrometries" presented at the National Center for Toxicological Research, Jefferson, AR, April 19, 2001.
- 28) P.B. Harrington, T.L. Buxton, G. Chen, and A.A. Urbas, "Chemometric Strategies for Ion Mobility and Mass Spectrometries" presented at Dow

Chemical, Midland, MI, March 17, 2001.

- 29) P.B. Harrington, "Making the Connection Between Neural Networks and Food Analysis" presented at Battelle Columbus, OH, May, 1998.
- 30) P.B. Harrington, "Making the Connection Between Neural Networks and Food Analysis" presented at Nabisco, East Hanover, NJ, May 14, 1996.
- 31) P.B. Harrington, "Ion Mobility Spectrometry Progress Report" presented to Light Weight Detection, U.S. Army, E.R.D.E.C., Edgewood, MD, April 16, 1996.
- 32) P.B. Harrington, "Making the Connection Between Neural Networks and Mass Spectrometry" presented at the FOM Institute for Molecular and Atomic Physics, Amsterdam, The Netherlands, August 2, 1995.
- 33) P.B. Harrington, P. Zheng, P. Tandler, and B. Wabuye, "Making the Connection: Neural Networks and Chemistry" presented at the National Center for Toxicological Research, Jefferson, AR, April 7, 1995.
- 34) D.A. Wuersig, B.W. Wabuye, and P.B. Harrington, "Cascade Correlation Neural Networks" presented at the Eastman Kodak Company, Rochester, NY, June 3, 1994.
- 35) P.B. Harrington, "Minimal Neural Networks," presented at Leybold Inficon, 2 Technology Place, East Syracuse, NY, March 1992.
- 36) P.B. Harrington, "Minimal Neural Networks," presented at the National Biscuit Company, East Hanover, NJ November, 1991.
- 37) P.B. Harrington, "Minimal Neural Networks," presented at Dow Chemical's Symposium on Neural Network Awareness, Dow Chemical, Freeport, TX, October 1991.
- 38) P.B. Harrington, "Minimal Neural Networks," The Experts in Automation Series, Consortium on Automated Analytical Laboratory Systems, National Institute of Standards and Technology, Gaithersburg, MD, August, 1991.
- 39) P.B. Harrington, "Intelligent Peptide Sequencing," presented at Applied Biosystems, Inc., Foster City, CA, February, 1991.
- 40) P.B. Harrington, "Fuzzy Rule-Building Expert Systems," presented at Charles Evans and Assoc., Redwood City, CA, February, 1991.
- 41) P.B. Harrington, "Partial Least Squares Analysis Applied to Property Prediction," presented at Nabisco Brands, Inc. East Hanover, NJ, December,

1989.

- 42) P.B. Harrington, "Survey of Pattern Recognition Methods," presented at Teledyne CME, Santa Clara, CA, December, 1989.
- 43) P.B. Harrington, "Demonstration of Resolve Software," U.S. Army CRDEC Quarterly Review of CBMS program, Edgewood, MD, November, 1989.

### Workshop Presentations

- 1) P.B. Harrington, "Data Pretreatment: Make it help and not hinder the analysis". In *Chemometrics for Forensic Scientists: The Good, the Bad, and the Misleading*, #15 at the American Academy of Forensic Sciences 62<sup>nd</sup> Annual Meeting, Seattle, WA, February 23, 2010.

### Presentations at International Scientific Conferences

(\*Denotes invited presentation and underlining the presenter)

- 1) P.P. Liu, X. Zhang, B.L. Pan, M.J. Wei, Z. Zhang, P.B. Harrington, "Classification of Sand Samples by using Terahertz Time-domain Spectroscopy and Chemometrics", *Colloquium Spectroscopicum Internationale XL*, 2017, Pisa, Italy, June 14, 2017.
- 2) P.B. Harrington\*, "Single Set Validation for Classification and Calibration Leads to False Conclusions", *International Congress on Analytical Sciences 2017*, Haikou, China, May 7, 2017, **Keynote**.
- 3) P.B. Harrington\*, "Single Set Validation for Classification and Calibration Causes False Conclusions", *5<sup>th</sup> Annual Congress of Analytix 2017*, Fukuoka, Japan, March 23, 2017, **Keynote**.
- 4) P.B. Harrington\*, "Bootstrapping as a Tool to Automate Chemometric Methods", *Chimétrie XVIII 2017*, Paris, France, January 30, 2017, **Plenary**.
- 5) P.B. Harrington, "Chemometric Shootout Method Used", *Chimétrie XVIII 2017*, Paris, France, January 30, 2017.
- 6) P.B. Harrington, "Parameter-Free Support Vector Machines for Calibration with Hybrid Penalty Functions", *XVI Chemometrics in Analytical Chemistry (CAC 2016)*, Barcelona, Spain, June 9, 2016.
- 7) P.B. Harrington\*, "Novel Multiclass Support Vector Machine Classification Tree Algorithm and its Application to Authentication of Traditional Chinese Medicines", *XV Chemometrics in Analytical Chemistry (CAC 2015)*, Changsha, PRC, June 25, 2015, **Keynote**.
- 8) Y. Li, B. Xiang, Y. Zong, G. Tang, L. Qu, Y. Wu, and P.B. Harrington, "Factor

Analysis of the Routine Components of Flue-cured Tobacco", *The 2014 International Conference on Computer Science and Software Engineering (CSSE 2014)*, Shenzhen, PRC, January 14, 2014.

- 9) P.B. Harrington\*, "Fuzzy Grid Encoding: A New Paradigm for Multivariate Chemometrics", *Analytix 2014*, Dalian, PRC, April 28, 2014, **Keynote**.
- 10) P.B. Harrington\*, "Smarter Products Based on Chemical Sensing", *World Emerging Industries Summit*, Wuhan, PRC, November 29, 2013, **Keynote**.
- 11) P.B. Harrington\*, "Fuzzy Optimal Associate Memories for Modeling Chemical Profiles: Authentication of Foods and Nutraceuticals", *The 1<sup>st</sup> International Symposium on Profiling 2013 (ISPROF-2013)*, Caparica, Portugal, September 3, 2013, **PL-4, Plenary**.
- 12) S.M. Cologna, P.S. Backlund, B.C. Searle, C.A. Wassif, P.B. Harrington, A.L. Yergey, F.D. Porter, "An iTRAQ Method to Assess Variability and Proteome Changes in Large Patient Cohorts: Application to Niemann-Pick disease, type C1", *The 60<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics*, Vancouver, CA, May 23, 2012, **WP046**.
- 13) Z. Wang, Y. Zhang, H. Zhang, P.B. Harrington, H. Chen, "Fast and Selective Modification of Thiol Proteins/Peptides by *N*-(Phenylseleno)phthalimide", *The 60<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics*, Vancouver, CA, May 22, 2012, **TP128**.
- 14) P.B. Harrington\*, "Fuzzy Optimal Associative Memories for the Authentication of Nutraceuticals by Mass Spectrometry", *The 6<sup>th</sup> Shanghai International Symposium on Analytical Chemistry*, Shanghai, PRC, October 16, 2012.
- 15) P.B. Harrington\*, "Authentication of Foods and Nutraceuticals", *6<sup>th</sup> International Forum on Food Safety*, Shanghai, PRC, September 29, 2011.
- 16) P.B. Harrington\*, "Fuzzy Entropy of Classification and Its Application to Biomarker Discovery: Application to Proteomics", *2009 Sixth International Conference on Fuzzy Systems and Knowledge Discovery*, Tianjin, PRC, August 16, 2009.
- 17) P.B. Harrington\*, "Fuzzy Entropy of Classification and Its Application to Biomarker Discovery: Algorithm", *2009 Sixth International Conference on Fuzzy Systems and Knowledge Discovery*, Tianjin, PRC, August 16, 2009.
- 18) P.B. Harrington, "Development of Nonlinear Modeling Methods for Chemical Agent Detection from Differential Mobility Images", *17<sup>th</sup> Annual Conference on Ion Mobility Spectrometry*, Ottawa, CA, July 24, 2008.

- 19) Z. Zhang\* and P.B. Harrington, "Identification of Rhubarbs by Using Near-infrared Spectrometry and Chemometric Methods", Colloquium Spectroscopicum Internationale XXXV, Xiamen, PRC, September 27, 2007.
- 20) P.B. Harrington\*, "Chemometric Opportunities in Proteomic Biomarker Discovery via Mass Spectrometry", Colloquium Spectroscopicum Internationale XXXV, Xiamen, PRC, September 24, 2007.
- 21) P.B. Harrington\*, "Chemometric Opportunities in Proteomic Biomarker Discovery via Mass Spectrometry", Fudan University Institutes of Biomedical Sciences Proteomics Pre-Conference, Shanghai, PRC, September 22, 2007, **Plenary**.
- 22) D. Melaragno, R. O'Donnell, P.B. Harrington\*, and S. Snyder, "Detection of Liquid and Cocktail Explosives by Ion and Differential Mobility Spectrometries", International Symposium on Analysis and Detection of Explosives, Paris, France, July 6, 2007.
- 23) P.B. Harrington, P. Chen, and A. Yergey, "Theoretical Foundations of Analysis of Variance-Principal Component Analysis", 10<sup>th</sup> International Conference on Chemometrics in Analytical Chemistry (CAC-2006), Aguas de Lindòia, Brazil, September 12, 2006.
- 24) P.B. Harrington\* and Y. Lu, "Forensic Applications of Chemometrics: Classification of Accelerants from Fire Debris by Gas Chromatography-Differential Mobility Spectrometry (GC-DMS)", 10<sup>th</sup> International Conference on Chemometrics in Analytical Chemistry (CAC-2006), Aguas de Lindòia, Brazil, September 12, 2006, **Keynote**.
- 25) P.B. Harrington\*, "Chemometric Opportunities in Proteomic Biomarker Discovery via Mass Spectrometry", 3<sup>rd</sup> Symposium on Computer Applications and Chemometrics in Analytical Chemistry (SCAC-2006), Lake Balaton, Hungary, July 5, 2006.
- 26) P. Rearden and P.B. Harrington, "Preprocessing of Gas Chromatography Differential Mobility Spectrometry (GC-DMS) Data for Curve Resolution and Classification of Fuels", 3<sup>rd</sup> Symposium on Computer Applications and Chemometrics in Analytical Chemistry (SCAC-2006), Lake Balaton, Hungary, July 4, 2006.
- 27) P. Reardon and P.B. Harrington, "Multiway Preprocessing of Gas Chromatography Differential Mobility Spectrometry (GC-DMS) Data for Curve Resolution of Jet Fuels", 14<sup>th</sup> International Conference on Ion Mobility Spectrometry, Maffliers, France, July 27, 2005.
- 28) P.B. Harrington, Leanna Kishler, and Ping Chen, "Data Fusion of Ion Mobility,



Flame Photometric, And Metal-Insulator-Metal Ensemble Measurements of Toxic Industrial Chemicals", 14<sup>th</sup> International Conference on Ion Mobility Spectrometry, Maffliers, France, July 25, 2005.

- 29) Z. Zhang\*, H. Zhou, S. Liu, and P.B. Harrington, "Application of Takagi-Sugeno Fuzzy System to the Classification of Cancer Patients Based on Elemental Contents in Serum Samples", International Conference on Chemometrics and Bioinformatics in Asia (CCBA-2004), Shanghai, China, October 19, 2004.
- 30) X. Cui, Z. Zhang, Y. Ren, S. Liu, and P.B. Harrington, "Quality Control of the Powder Pharmaceutical Samples of Sulfaguanidine Based on NIR Reflectance Spectra with Temperature-Constrained Cascade Correlation Neural Networks", International Conference on Chemometrics and Bioinformatics in Asia (CCBA-2004), Shanghai, China, October 16, 2004.
- 31) P.B. Harrington\*, M.L. Ochoa, N.E. Vieira, and A.L. Yergey, "Chemometric Approaches to Mass Spectrometry of the Proteome: Modeling MALDI-MS", International Conference on Chemometrics and Bioinformatics in Asia (CCBA-2004), Shanghai, China, October 16, 2004.
- 32) P.B. Harrington\*, M.L. Ochoa, N.E. Vieira, A.L. Yergey, "Chemometric Considerations in Proteomic Analyses by Mass Spectrometry", Chemometrics and Analytical Chemistry 2004, Lisbon, Portugal, September 20, 2004.
- 33) P.B. Harrington and Libo Cao, "Modeling Nonlinear Wavelet Compressed Ion Mobility Spectrometry", 12<sup>th</sup> International Conference on Ion Mobility Spectrometry, Umeå, Sweden, July 28, 2003.
- 34) P.B. Harrington and Libo Cao, "Tutorial on Modeling and Wavelet Compression for Ion Mobility Spectrometrists", 12<sup>th</sup> International Conference on Ion Mobility Spectrometry, Umeå, Sweden, July 28, 2003.
- 35) Z. Zhang\*, H. Zhou, S. Liu, and P.B. Harrington, "Classification of Cancer Patients Based on ICP-AES Determinations Using Neural Networks", 9<sup>th</sup> Beijing Conference and Exhibition on Instrumental Analysis, Beijing, PRC, 2001.
- 36) P.B. Harrington, T.L. Buxton, and G. Chen, "Classification of Bacteria by Thermal Methylation Hydrolysis Ion Mobility Spectrometry Using SIMPLISMA and Multidimensional Wavelet Compression", Tenth International Conference on Ion Mobility Spectrometry, Wernigerode, Germany, August 15, 2001.
- 37) P.B. Harrington\*, T.L. Buxton, G. Chen, P.J. Rauch, L. Shaw, and A. Urbas, "Strategies for Smarter Chemical Sensors", 7<sup>th</sup> International Conference on Chemometrics in Analytical Chemistry, Antwerp, Belgium, October 20, 2000.

- 38) P.B. Harrington, T.L. Buxton, G. Chen, P.J. Rauch, L. Shaw, and A. Urbas, "Chemometric Strategies for Smarter Ion Mobility Spectrometers", 9<sup>th</sup> International Symposium on Ion Mobility Spectrometry, Halifax, Canada, August 15, 2000.
- 39) T. Buxton and P.B. Harrington, "Modified Ion Mobility Spectrometer for Enhanced Selectivity", 26<sup>th</sup> Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Vancouver, BC, Canada, October 28, 1999, **705**.
- 40) P.B. Harrington\*, J. Wan, C. Cai, and A. Urbas, "Applications of Neural Networks to Environmental Analysis", 26<sup>th</sup> Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Vancouver, BC, October 27, 1999, **487**.
- 41) P.B. Harrington\* and J. Wan, "Sensitivity Analysis Applied to Artificial Neural Networks: What has my neural network actually learned?", 8<sup>th</sup> International Symposium on Ion Mobility Spectrometry, Buxton, United Kingdom, August 9, 1999.
- 42) P.B. Harrington, "Temperature Constrained-Cascade Correlation Networks", 5<sup>th</sup> Scandinavian Chemometrics Conference, Lahti, Finland, August 26, 1997.
- 43) P.B. Harrington, E.S. Reese, P.J. Rauch, C. Wan, and D.M., Davis, "Chemometric Tools for Advantageous Use of Dynamic IMS Data", 6<sup>th</sup> International Symposium on Ion Mobility Spectrometry, Bastei, Germany, August 14, 1997.
- 44) P.B. Harrington\* and L. Hu, "Copiosity Principle for 21st Century Chemometricians", Chemometrics in Analytical Chemistry, Tarragona, Spain, June 25, 1996.
- 45) P. Johnson, L. Hu, E Saulinskas, and P.B. Harrington, "An Expert System for Amino Acid Sequence Analysis", XI<sup>th</sup> International Conference on Methods in Protein Structure Analysis, Annecy, FR, September 3, 1996.
- 46) P.B. Harrington\*, P. Zheng, and Dennis Davis, "Automatic Deconvolution-Temperature Constrained Cascade Correlation Neural Networks for Ion Mobility Data Analysis", 4<sup>th</sup> International Workshop on Ion Mobility Spectrometry, Cambridge, United Kingdom, August 7, 1995.
- 47) P.B. Harrington\*, "Minimal Neural Networks", Compana-1992, Jena, Germany, August 25, 1992.
- 48) P.B. Harrington\* and B.W. Pack, "FLIN: Fuzzy Linear Interpolating Network", Chemometrics in Analytical Chemistry-1992, Montreal, Quebec, Canada, July 1992.

**Presentations at U.S. Scientific Conferences**

(\*Denotes invited presentation and underlining the presenter)

- 1) X. Wang, P.B. Harrington, and S.F. Baugh, "Comparative Study of Nuclear Magnetic Resonance Spectral Profiling for the Characterization of *Cannabis*", Practical Applications of NMR in Industry Conference (PANIC 2017), Hilton Head, SC, February 20-22, 2017.
- 2) P.B. Harrington, "Automatic Support Vector Machines for Calibration with 3 Different Loss Functions", Federation of Analytical Chemistry and Spectroscopy Societies, SciX 2016, Minneapolis, MN, September, 19, 2016, 778 (fill-in).
- 3) P.B. Harrington\*, "Automatic Support Vector Machines for Calibration with Differential Penalty Functions", Federation of Analytical Chemistry and Spectroscopy Societies SciX 2016, Minneapolis, MN, September, 19, 2016, 163.
- 4) X. Wang, P.B. Harrington, and S.E. Baugh, "Comparative Study for the Authentication of Marijuana Varieties by Conventional and High-Resolution Mass Spectrometric Profiling". The 64<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Antonio, TX, June 9, 2016, ThOA.
- 5) X. Wang, P.B. Harrington, and S.F. Baugh, "Comparative Study for the Authentication of Marijuana Varieties by Conventional and High-Resolution Mass Spectrometric Profiling", 2016 Ohio University Student Research and Creative Activity Expo, Athens, OH, April 14, 2016.
- 6) A.K. Aloglu, P.B. Harrington, S. Sahin, and C. Demir, "Prediction of Total Antioxidant Activity of *Prunella* L. Species by Automatic Partial Least Square Regression Applied to 2-Way Liquid Chromatographic UV Spectral Images", 2016 Ohio University Student Research and Creative Activity Expo, Athens, OH, April 14, 2016.
- 7) P.B. Harrington, X. Wang, S.E. Baugh, D.E. Anderson, and J.D. McChesney, "Novel Three-Dimensional Chemical Characterization and Visualization Tool Applied to Green Tea, Hops, and Cannabis Varieties", The 16<sup>th</sup> Annual Oxford International Conference on the Science of Botanicals 5th Interim American Society of Pharmacognosy Meeting (ICSB 2016), Oxford, MS, April 11, 2016.
- 8) P.B. Harrington\*, "Chemometric Strategies for Authenticating Botanical Reference Materials", BERM: International Symposium on Biological and Environmental Reference Materials, National Harbor, MD, October 15, 2015.
- 9) P.B. Harrington\*, X. Wang, S.E. Baugh, "Comparative Study of Classification Trees for the Authentication of Marijuana", Federation of Analytical Chemistry

and Spectroscopy Societies SciX 2015, September, 28, 2015.

- 10) P.B. Harrington\*, "Novel Multiclass Support Vector Machine Classification Tree Algorithm and its Application to Authentication of Traditional Chinese Medicines", *XV Chemometrics in Analytical Chemistry (CAC 2015)*, Changsha, PRC, June 25, 2015, **Keynote**.
- 11) J. Harnly, P. Chen, K. Colson, J.A. McCoy, D.H. Reynaud, and P.B. Harrington "MS, NMR, and DNA barcoding, complementary methods for identification and authentication of Black Cohosh (*Actaea racemosa* L.)", American Society of Pharmacognosy Annual Meeting, Copper Mountain, CO, July 25, 2015, **1014**.
- 12) X. Wang and P.B. Harrington, "Differentiating Rice Varieties by SPME-GC-MS and NMR Chemical Profiling", The 63<sup>RD</sup> ASMS Conference on Mass Spectrometry and Allied Topics, St. Louis, MO, June 9, 2015, **TP 328**.
- 13) X. Wang and P.B. Harrington, "Differentiating Rice Varieties by SPME-GC-MS and NMR Chemical Profiling", Ohio University Student Research & Creative Expo, Athens, OH, April 9, 2015, **161**.
- 14) M. Zhang and P.B. Harrington, Field Analysis of Trichloroethylene in Water using Liquid-liquid Microextraction Assisted Solid Phase Microextraction with Portable Gas Chromatography/Mass Spectrometry. Federation of Analytical Chemistry and Spectroscopy Societies SciX 2014 Conference. Reno, NV, September 29, 2014, **119**.
- 15) P. Scholl, S. Farris, R. Romero, P.B. Harrington, J. Moore, and P. Lutter, "MALDI-TOF-MS Screening of Skim Milk Powder for Economically Motivated Adulteration with Foreign Proteins: An Inter-laboratory Feasibility of Concept Demonstration", The 62<sup>nd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Baltimore, MD, June 19, 2014, **Th 610**.
- 16) M. Zhang, and P.B. Harrington, "Determination of Aroclor 1254 and 1260 in Soil Samples by Headspace Solid Phase Microextraction - GC/MS using Partial Least-Squares Regression", The 62<sup>nd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Baltimore, MD, June 19, 2014, **Th 561**.
- 17) X. Wang, and P.B. Harrington, "Differentiating Rice Varieties by Inductively Coupled Plasma/Mass Spectrometry Chemical Profiling", The 62<sup>nd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Baltimore, MD, June 18, 2014, **W 343**.
- 18) Z. Wang, M. Zhang, and P.B. Harrington, "Reconstruction of Mass Spectra Using Fuzzy Optimal Associative Memories (FOAMs)", The 62<sup>nd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Baltimore, MD, June 18,

2014, **W 026**.

- 19) X. Wang and P.B. Harrington, "Differentiating Rice Varieties by Inductively Coupled Plasma—Mass Spectrometry Chemical Profiling", Ohio University Student Research & Creative Expo, Athens, OH, April 10, 2014.
- 20) M. Zhang and P.B. Harrington, "Determination of Aroclor 1254 and 1260 in Soil Samples by Headspace Solid Phase Microextraction – GC/MS using Partial Least-Squares Regression", Ohio University Student Research & Creative Expo, Athens, OH, April 10, 2014.
- 21) A.H. Banirashaid, P.B. Harrington, and G.P. Jackson, "Amino Acid Composition of Human Scalp Hair as a Biometric Classifier and Investigative Lead", The 2<sup>nd</sup> International Conference on Forensic Research and Technology, Las Vegas, NV, October 8, 2013, **974**.
- 22) M. Zhang, P.B. Harrington, N.A. Kruse, J.R. Bowman, S.A. Lammert, E.D. Lee, and G.P. Jackson, "Development of an Expedited Field Study Method for PCBs in Sediments and Soils Using Portable GC/MS", The 61<sup>st</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Minneapolis, MN, June 13, 2013, **ThP 187**.
- 23) Z. Wang, P. Chen, L. Yu, and P.B. Harrington. "Authentication of organic basil plants by using gas chromatography/mass spectrometry chemical profiles", The 61<sup>st</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Minneapolis, MN, June 13, 2013, **ThP 186**.
- 24) M. Zhang, P.B. Harrington, N.A. Kruse, J.R. Bowman, S.A. Lammert, E.D. Lee, and G.P. Jackson, "Development of an Expedited Field Study Method for PCBs in Sediments and Soils Using Portable GC/MS", Ohio University Student Research & Creative Expo, Athens, OH, April 11 2013, **CheBio-G3 21**.
- 25) Z. Wang, P. Chen, L. Yu, and P.B. Harrington. "Authentication of organic basil plants by using gas chromatography/mass spectrometry chemical profiles", Ohio University Student Research & Creative Expo, Athens, OH, April 11 2013, **CheBio-G3 32**.
- 26) Z. Wang, Y. Zhang, H. Zhang, P.B. Harrington, H. Chen, "Fast and Selective Modification of Thiol Proteins/Peptides by *N*-(Phenylseleno)phthalimide", OHIO University Research and Creative Activity Expo, Athens, OH, May 14, 2012, **12**.
- 27) W. Lu, G.J. Rankin, A. Bondra, C. Trader, A. Heeren, and P.B. Harrington, "Gasoline and Kerosene Identifications Using Two-way Gas Chromatography/Mass Spectrometry by Chemometric Analysis", OHIO University Research and Creative Activity Expo, May 13, 2011, **188**.

- 28) X. Sun, P. Chen, S. Cook, G.P. Jackson, and P.B. Harrington, "Classification of Cultivation Locations of *Panax quinquefolium* (American Ginseng) using Chemometrics and High Performance Liquid Chromatography/Electrospray-Mass Spectrometry", OHIO University Research and Creative Activity Expo, May 13, 2011, **325**.
- 29) Z. Xu, X. Sun, and P.B. Harrington, "Baseline Correction Method Using an Orthogonal Basis for Gas Chromatography/Mass Spectrometry", OHIO University Research and Creative Activity Expo, May 13, 2011, **332**.
- 30) P.B. Harrington\*, "Chemometric Opportunities for Ion Mobility and Mass Spectrometries", Pittsburgh Mass Spectrometry Discussion Group, Pittsburgh, PA, October 5, 2010.
- 31) P.B. Harrington\*, "Chemometric Strategies for Authentication of Foods and Herbal Supplements", 124<sup>th</sup> AOAC Meeting and Exhibition, Orlando, FL, September 29, 2010.
- 32) X. Sun, Z. Miao, P.B. Harrington, J. Colla, and H. Chen, "Coupling of Single-Droplet Liquid-Liquid-Liquid Micro-Extraction with Desorption Electrospray Ionization Mass Spectrometry", OHIO University Research and Creative Activity Expo, May 13, 2010, **138**.
- 33) Z. Xu, C.E. Bunker, and P.B. Harrington, "Classification of Jet Fuel Properties by Near Infrared Spectroscopy Using Fuzzy Rule-Building Expert Systems and Support Vector Machines", OHIO University Research and Creative Activity Expo, May 13, 2010, **041**.
- 34) W. Lu, J.H. Callahan, F.S. Fry, S.M. Musser and P.B. Harrington, "Discriminant Based Charge Deconvolution Approach for Liquid Chromatography Electrospray Ionization Mass Spectrometry", OHIO University Research and Creative Activity Expo, May 13, 2010, **045**.
- 35) P.B. Harrington\*, W. Lu, and Y. Lu, "Novel Algorithm for Registration of Hyperspectral Images and Retention Time Alignment of Multiway Data", 36<sup>th</sup> Federation of Analytical Chemistry and Spectroscopy Societies, Louisville, KY, October 22, 2009.
- 36) J. Harnly, P. Chen, and P.B. Harrington, "Discrimination between Asian and American Ginseng using a Methanol:Water Extraction, UV Spectrophotometry, and Pattern Recognition Analysis", 123<sup>rd</sup> Association of Analytical Communities (AOAC) International Annual Meeting & Exposition, Philadelphia, PA, September 14, 2009.
- 37) Yao Lu and P.B. Harrington, "Comparison of DMS and MS for Gas Chromatographic Detection of Ignitable Liquids from Fire Debris Using PDR",

- OHIO University Research and Creative Activity Expo, May 14, 2009, **201**.
- 38) Zhanfeng Xu and P.B. Harrington, "Classification and Prediction of Jet Fuel Properties by Near Infrared Spectroscopy", OHIO University Research and Creative Activity Expo, May 14, 2009, **155**.
  - 39) Weiyang Lu and P.B. Harrington, "Radial Basis Function Cascade Correlation Networks", OHIO University Research and Creative Activity Expo, May 14, 2009, **64**.
  - 40) Xiaobo Sun and P.B. Harrington, "Classification of Jet Fuels by Fuzzy Rule-Building Expert Systems Applied to Two-Way Fast GC Fast/MS Data", OHIO University Research and Creative Activity Expo, May 14, 2009, **049**.
  - 41) Y. Lu and P.B. Harrington\*, "Comparison of Differential Mobility Spectrometry and Mass Spectrometry for Gas Chromatography and Two-way Classification of Ignitable Liquids from Fire Debris", 35<sup>th</sup> Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Reno, NV, September 30, 2008.
  - 42) R.M. O'Donnell and P.B. Harrington, "Detection of Cocaine & Marijuana Metabolites in Adulterated Urine", OHIO University Research and Creative Activity Expo, May 15, 2008, **031**.
  - 43) Y. Lu and P.B. Harrington, "Detection of Drug Metabolites in Urine Using Solid Phase Extraction and Ion Mobility Spectrometry with Alternating Least Squares", OHIO University Research and Creative Activity Expo, May 15, 2008, **549**.
  - 44) W. Lu and P.B. Harrington, "Theory and Analytical Applications of the Temperature Constrained Radial Basis Function Neural Networks", the 59<sup>th</sup> Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), New Orleans, LA, March 7, 2008, **2530-7**.
  - 45) R.M. O'Donnell and P.B. Harrington, "Detection of Marijuana and Cocaine Metabolites in Adulterated Urine Using Solid Phase Extraction-Ion Mobility Spectrometry and Gas Chromatography-Mass Spectrometry", the 59<sup>th</sup> Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), New Orleans, LA, March 6, 2008, **2200-8**.
  - 46) X. Sun, P.B. Harrington, C.M. Zimmerman, G.P. Jackson, and C.E. Bunker, "Classification of Jet Fuel Physical Properties by Fuzzy Rule-Building Expert Systems Applied to Two-Way Fast GC-Fast MS Data Objects", the 59<sup>th</sup> Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), New Orleans, LA, March 6, 2008, **1930-3**.

- 47) P. Chen, Y. Lu, and P.B. Harrington, "Classification of Accelerants by Gas Chromatography-Differential Mobility Spectrometry and Temperature Constraint Cascade Correlation Neural Networks", the 59<sup>th</sup> Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), New Orleans, LA, March 5, 2008, **1490-8**.
- 48) Y. Lu and P.B. Harrington, "Rapid and Facile Detection of Stimulants and Their Metabolites in Urine Using Solid Phase Extraction-Thermal Desorption-Ion Mobility Spectrometry with Alternating Least Squares", the 59<sup>th</sup> Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), New Orleans, LA, March 5, 2008, **1440-2**.
- 49) D. Melaragno and P.B. Harrington, "Detection of Liquid and Cocktail Explosives by Ion Mobility Spectrometry", the 59<sup>th</sup> Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), New Orleans, LA, March 5, 2008, **1170-3**.
- 50) Z. Xu, C.E. Bunker, and P.B. Harrington, "Classification and Prediction of Jet Fuel Properties by Near Infrared Spectroscopy", the 59<sup>th</sup> Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), New Orleans, LA, March 4, 2008, **430-5**.
- 51) P.B. Harrington\*, Y. Lu, and P. Chen, "Ion and Differential Mobility Spectrometries: Portable Tools for Forensic Investigations", Central Regional Meeting of the American Chemical Society (CERMACS-2007), Covington, KY, May 28, 2007, **107**.
- 52) D. Melaragno, P.B. Harrington, and S. Snyder, "Detection of Liquid and Cocktail Explosives by Ion Mobility and Gas Chromatography Mass Spectrometries", Central Regional Meeting of the American Chemical Society (CERMACS-2007), Covington, KY, May 27, 2007, **542**.
- 53) R.M. O'Donnell, X. Sun, and P.B. Harrington, "Applications of Ion Mobility Spectrometry and Differential Mobility Spectrometry in Drug Screening and Quality Control of Pharmaceuticals", Central Regional Meeting of the American Chemical Society (CERMACS-2007), Covington, KY, May 27, 2007, **41**.
- 54) P. Chen and P.B. Harrington, "Nonlinear Discrete Wavelet Compression of MALDI-MS Spectra for Classification of Pathogenic Foodborne Bacteria", OHIO University Research and Creative Activity Expo, May 3, 2007.
- 55) Y. Lu and P.B. Harrington, "Two-Way Classification of Pathogenic Bacteria by Fast Gas Chromatography Mass Spectrometry Analysis of Fatty Acid Methyl Esters", OHIO University Research and Creative Activity Expo, May 3, 2007.
- 56) Y. Lu and P.B. Harrington, "Two-way Data Classification of Foodborne



Pathogenic Bacteria by Fast Gas Chromatography-Mass Spectrometry Analysis of Fatty Acid Methyl Esters", the 58th Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2007), Chicago, IL, February 28, 2007, **1640-8**.

- 57) P. Chen and P.B. Harrington, "Nonlinear Discrete Wavelet Compression of MALDI-MS Spectra for Classification of Foodborne Bacteria", the 58th Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2007), Chicago, IL, February 28, 2007, **220-16P**.
- 58) P.B. Harrington and Y. Lu, Forensic Applications of Chemometrics: Statistical Comparison of Differential and Ion Mobility Spectrometry for Gas Chromatographic Detection and Three-Way Classification of Ignitable Liquids from Fire Debris, The American Academy of Forensic Sciences 59<sup>th</sup> Annual Meeting, San Antonio, TX, February 24, 2007, **B194**.
- 59) P.B. Harrington\*, Y. Lu, P. Chen, J.J. Karnes, and C.E. Bunker, "Classification Of Two-way Data for Forensic Fingerprinting of Fuels by Chromatography-Mass Spectrometry and Gas Chromatography-Differential Mobility Spectrometry" presented at The 33<sup>rd</sup> Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Lake Buena Vista, FL, September 27, 2006.
- 60) P.B. Harrington\*, "Two-way Multivariate Correlation as an Information Theoretic Tool for Measuring Analytical Orthogonality" presented at The 33<sup>rd</sup> Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Lake Buena Vista, FL, September 25, 2006.
- 61) P.B. Harrington and Yao Lu, "Forensic Applications of Chemometrics: Classification of Accelerants from Fire Debris by Gas Chromatography-Differential Mobility Spectrometry (GC-DMS)", presented at The 15<sup>th</sup> International Conference on Ion Mobility Spectrometry, Honolulu, HI, July 27, 2006.
- 62) P.B. Harrington\*, "Chemometric Opportunities in Proteomic Biomarker Discovery via Mass Spectrometry", presented at the inaugural Ohio Collaborative Conference on Bioinformatics (OCCBIO), Athens, Ohio, June 29, 2006.
- 63) A.L. Yergey\*, P.B. Harrington, N.E. Vieira, R. Romero, "Analysis of Variance-Principal Component Analysis: A Soft Tool for Proteomic Discovery of MALDI-MS Biomarkers from Amniotic Fluid", presented at the 54<sup>th</sup> ASMS Conference on Mass Spectrometry, Seattle, WA, June 26, 2006.
- 64) P. Chen and P.B. Harrington, "Identification of Toxic Industrial Chemicals Using dual Ion Mobility Spectrometry and Multivariate Pattern Recognition

Algorithms”, OHIO University Research and Creative Activity Expo, May 4, 2006.

- 65) Y. Lu and P. B. Harrington, “Forensic Analysis of Accelerants in Fire Debris by Gas Chromatography-Differential Mobility Spectrometry (GC-DMS) and Pattern Recognition”, OHIO University Research and Creative Activity Expo, May 4, 2006.
- 66) P.B. Harrington\*, “Ion and Differential Mobility Spectrometries: Portable Tools for Crime Scene Investigations”, presented at the 115<sup>th</sup> Annual Meeting of The Ohio Academy of Science, Dayton, OH, April 22, 2006.
- 67) P. Chen and P.B. Harrington, “Comparison of Temperature-Constrained Cascade Correlation Networks and a Fuzzy Rule-Building Expert System for Identification of Toxic Compounds Using Dual Scan Ion Mobility Data”, presented at The 57<sup>th</sup> Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 16, 2006, **2330-1**.
- 68) P. Rearden and P.B. Harrington, “Preprocessing of Gas Chromatography Differential Mobility Spectrometry (GC-DMS) Data for Curve Resolution and Classification of Fuels”, presented at The 57<sup>th</sup> Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 16, 2006, **2100-17**.
- 69) L.N. Kishler and P.B. Harrington, “Sensor Fusion for Detection of Toxic Industrial Chemicals”, presented at The 57<sup>th</sup> Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 16, 2006, **2100-9**.
- 70) Y. Lu and P.B. Harrington, “Classification of Accelerants from Fire Debris by Gas Chromatography-Differential Mobility Spectrometry (GC-DMS) and Pattern Recognition”, presented at The 57<sup>th</sup> Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 14, 2006, **1160-8**.
- 71) P.B. Harrington, Ping Chen, Preshious Rearden, and Yao Lu, “Chemometric Opportunities in Forensic Chemical Analysis”, presented at The 57<sup>th</sup> Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 13, 2006, replaced **580-2580-3**.
- 72) P.B. Harrington\*, P. Rearden, P. Chen, J.J. Karnes, and C.E. Bunker, “Two-way Multivariate Correlation a Measure of Orthogonality and a Comparison to Multivariate Curve Resolution” presented at The 57<sup>th</sup> Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 13, 2006, **580-1**.

- 73) L. Kishler and P.B. Harrington, "Data Fusion of Ion Mobility, Flame Photometric, and Metal-Insulator-Metal Ensemble Measurements of Toxic Industrial Chemicals", presented at the American Academy of Forensic Sciences 58th Annual Meeting, Seattle, WA, February 21, 2006.
- 74) P. Rearden and P.B. Harrington, "Multiway Preprocessing of Gas Chromatography Differential Mobility Spectrometry (GC-DMS) Data for Curve Resolution of Jet Fuels", presented at the Sigma Xi Annual Meeting and Student Research Conference, Seattle, WA, November 4, 2005.
- 75) P. Rearden and P.B. Harrington, "Rapid Screening of Precursor and Degradation Products of Chemical Warfare Agents in Soil by Solid-Phase Microextraction Ion Mobility Spectrometry (SPME-IMS)", OHIO University Research and Creative Activity Expo, May 12, 2006.
- 76) P. Chen and P.B. Harrington, "Multivariate Modeling of Dual Scan Ion and Differential Mobility Spectra", presented at The 56th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 3, 2005, **1710-1**.
- 77) P. Rearden and P.B. Harrington, "Photoionization Differential Ion Mobility Spectrometer as a Gas Chromatographic Detector for Volatile Organic Compounds" presented at The 56th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 1, 2005, **650-7**.
- 78) P.B. Harrington\*, P. Chen, and M.L. Ochoa, "Fuzzy Entropy Classification Systems and Their Application to Mass Spectrometry of the Proteome", presented at the Mathematical Biosciences Institute Workshop 3 Computational Proteomics and Mass Spectrometry, Columbus, OH, January 11, 2005.
- 79) A.L. Yergey\*, P.B. Harrington, N.E. Vieira, and R. Romero, "Mass Spectrometric Profiling for Disease Diagnosis: Development of Methodology", presented at the Mathematical Biosciences Institute Workshop 3 Computational Proteomics and Mass Spectrometry, Columbus, OH, January 11, 2005.
- 80) P. Chen\* and P.B. Harrington, "ANOVA-PCA Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry of Microorganisms", presented at the Mathematical Biosciences Institute Workshop 3 Computational Proteomics and Mass Spectrometry, Columbus, OH, January 12, 2005.
- 81) P.B. Harrington and P. Chen, "Equilibrium Modeling of Ion Mobility Spectra", presented at The 13<sup>th</sup> International Conference on Ion Mobility Spectrometry,

Gatlinburg, TN, July 29, 2004.

- 82) M.L. Ochoa and P.B. Harrington, "Chemometric Studies for the Characterization and Differentiation of Food borne Bacteria Pathogens by Thermal Desorption Ion Mobility Spectrometry", presented at The 13<sup>th</sup> International Conference on Ion Mobility Spectrometry, Gatlinburg, TN, July 25, 2004.
- 83) P. Rearden and P.B. Harrington, "Solid Phase Microextraction Ion Mobility Spectrometry for the Selective Detection of Volatile Aldehydes", presented at The 31<sup>st</sup> Annual Conference of the National Organization of the Professional Advancement of Black Chemists and Chemical Engineers, San Diego, CA, April 13, 2004.
- 84) M.L. Ochoa and P.B. Harrington, "Characterization of Food-borne Bacterial Pathogens by MALDI-TOF MS and IMS", presented at The Annual Meeting of the Ohio Branch of the American Society of Microbiology, Youngstown, OH, April 17, 2004.
- 85) E.A. Gombas and P.B. Harrington, "Optimization of Ion Mobility Spectrometry of *Escherichia coli* Strains", presented at The Annual Meeting of the Ohio Branch of the American Society of Microbiology, Youngstown, OH, April 17, 2004.
- 86) P.B. Harrington\*, M.L. Ochoa, S.P. Markey, C. Laurent, K. Saito, and A.L. Yergey, "Chemometric Considerations in Proteomic Analyses by Mass Spectrometry", presented at the Institute for Pure and Applied Mathematics, Los Angeles, CA, March 22, 2004.
- 87) P. Rearden and P.B. Harrington, "Solid Phase Microextraction Ion Mobility Spectrometry for the Selective Detection of Volatile Aldehydes", presented at The 55th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Chicago, IL, March 12, 2004, **25700-500**.
- 88) M.R. Rainsberg and P.B. Harrington, "A Novel Solid Phase Microextraction Inlet System for the Detection of Volatile Organic Compounds by Differential Mobility Spectrometry", presented at The 55th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Chicago, IL, March 11, 2004, **23300-700**.
- 89) E.A. Gombas and P.B. Harrington, "Optimization of Ion Mobility Spectrometry of *Escherichia coli* Strains", presented at The 55th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Chicago, IL, March 10, 2004, **15900-500**.
- 90) M.L. Ochoa and P.B. Harrington, "Characterization of Food-borne Bacterial

Pathogens by MALDI-TOF MS and IMS”, presented at The 55th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Chicago, IL, March 10, 2004, **14900-800**.

- 91) L. Cao and P.B. Harrington, “SIMPLISMA and ALS Applied to Nonlinear Wavelet Compressed Ion Mobility Spectra of Chemical Warfare Simulants”, presented at The 55th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Chicago, IL, March 9, 2004, **14600-100**.
- 92) P.B. Harrington and L. Cao, “Chemometric Modeling of Mass Spectra”, presented at the 2<sup>nd</sup> Ohio Analytical Chemistry Consortium, Columbus, OH, October 31, 2003.
- 93) A.K. Gianatto, J.W. Rawlinson, K.C. Cossel, P.B. Harrington, A.D. Appelhans, R. Tandy, S. Gowatham, and G.S. Groenewold, “Formation and Hydration on Aluminum Oxide Cluster Ions in a Quadrupole Ion Trap”, presented at The 29<sup>th</sup> Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Ft. Lauderdale, FL, October 21, 2003.
- 94) M.L. Ochoa and P.B. Harrington, “Detection of Methamphetamine in the Presence of Nicotine Using Derivatization and Ion Mobility Spectrometry” presented at The 54th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 12, 2003, **2520-5**.
- 95) L. Cao, P.B. Harrington, and G. Chen, “Histogram Mass Spectra Lose Key Chemical Information: Are Wavelet Compressed Mass Spectral Profiles a Viable Alternative?” presented at The 54th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 12, 2003, **1770-8P**.
- 96) P. Rearden, P.B. Harrington, and K. Daum, “Selective Detection of Volatile Analytes Using Ion Mobility Spectrometry and Chemical Derivatization” presented at The 54th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 11, 2003, **1220-16P**.
- 97) L. Cao, P.B. Harrington, and G. Chen, “Wavelet Compressed Mass Spectral Profiles Perform as Better Alternative to Histogram Mass Spectra” presented at The 54th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 10, 2003, **730-1**.
- 98) P.B. Harrington\*, “Chemometrics Opportunities in Ion Mobility and Mass Spectrometries” presented at The 1st Ohio Analytical Chemistry Consortium, Columbus, OH, November 8, 2002.
- 99) L. Cao, G. Chen, and P.B. Harrington, “Histogram Mass Spectra Lose Key Chemical Information: Are Wavelet Compressed Mass Spectral Profiles a

Viable Alternative?" presented at The 1st Ohio Analytical Chemistry Consortium, Columbus, OH, November 8, 2002.

- 100) P.B. Harrington, A.K. Gianotto, B.D.M. Hodges, A.D. Appelhans, J.E. Olson, M.T. Benson, and G.S. Groenewold\*, "Chemometric Modeling Condensation of Reactions of  $\text{Cr}_x\text{O}_y^-$  in an Ion Trap Secondary Ion Mobility Spectrometer" presented at The 1<sup>st</sup> Ohio Analytical Chemistry Consortium, Columbus, OH, November 8, 2002.
- 101) A.K. Gianotto, B.D.M. Hodges, A.D. Appelhans, J.E. Olson, M.T. Benson, P.B. Harrington, and G.S. Groenewold\*, "Modeling Condensation of Reactions of  $\text{Cr}_x\text{O}_y^-$  in an Ion Trap Secondary Ion Mobility Spectrometer" presented at The 29<sup>th</sup> Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Providence, RI, October 15, 2002, **330**.
- 102) P.B. Harrington\*, T.L. Buxton, and G. Chen, "Real-time Chemometrics Applied to Screening Food Borne Pathogens and Biomarkers Using Ion Mobility Spectrometry: Chemometrics<sup>N</sup>" presented at the 2002 Chemometrics in Analytical Chemistry Meeting, Seattle, WA September 25, 2002.
- 103) M. Elena Velasquez, P.B. Harrington, and K. Bosworth, "Automated Assays of Radionuclides in Chemical Waste by Passive Gamma-ray Spectroscopy and Chemometrics presented at the 2002 Chemometrics in Analytical Chemistry Meeting, Seattle, WA September 23-24, 2002.
- 104) P.B. Harrington\*, G. Chen, and N.L. Schmitt, "Detection of Biogenic Amines in Foods Using Ion Mobility Spectrometry and Chemometrics" presented at the 224<sup>th</sup> American Chemical Society National Meeting, Boston, MA, August 20, 2002, **192**.
- 105) A.K. Gianotto, B.D.M. Hodges, A.D. Appelhans, P.B. Harrington, G.S. Groenewold, M. T. Benson, "Oxidation of  $\text{Cr}_x\text{O}_y^-$  in an Ion Trap Secondary Ion Mass Spectrometer", The 50th ASMS Conference on Mass Spectrometry and Allied Topics, Orlando, FL, June 6, 2002, **ThPQ360**.
- 106) P.B. Harrington, J. Rees, and K.J. Voorhees, "Classification of Food Borne Pathogens and their Mixtures by MALDI-MS and Wavelet Compressed Inverse Least Squares Regression", The 50th ASMS Conference on Mass Spectrometry and Allied Topics, Orlando, FL, June 4, 2002, **TPK291**.
- 107) L. Cao, G. Chen, and P.B. Harrington, "Histogram Mass Spectra Lose Key Chemical Information: Are Wavelet Compressed Mass Spectral Profiles a Viable Alternative?", The 50th ASMS Conference on Mass Spectrometry and Allied Topics, Orlando, FL, June 3, 2002, **MPK349**.
- 108) T.L. Buxton and P.B. Harrington, "Detection of Illegal Narcotics and Their

- Metabolites in Urine Using Solid-Phase Extraction Ion Mobility Spectrometry (SPE-IMS)", The 53rd Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, New Orleans, LA, March 20, 2002, **1339**.
- 109) G. Chen and P.B. Harrington, "Detection of Heroin in Drugs of Abuse Using Multivariate Curve Resolution with Two-Dimensional Wavelet Compression", The 53rd Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, New Orleans, LA, March 20, 2002, **889**.
- 110) G. Chen and P.B. Harrington, "Real-time Self-modeling Mixture Analysis with Wavelet Compression for Detection of Explosives Using an Ion Trap Mobility Spectrometer", The 53 Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, New Orleans, LA, March 20, 2002, **2126P**.
- 111) P.B. Harrington\*, T.L. Buxton, and G. Chen, "Chemometric Strategies for Smart Ion Mobility and Mass Spectrometries," The 115<sup>th</sup> AOAC INTERNATIONAL Annual Meeting, Kansas City, MO, September 11, 2001.
- 112) P.B. Harrington\*, A.A. Urbas, K.J. Voorhees, and J. Rees, "Wavelet Compression and De-noising of MALDI-MS Measurements of Bacteria," The 49<sup>th</sup> American Society for Mass Spectrometry Conference, Chicago, IL, May 31, 2001, **ThOCpm**.
- 113) A. Mehay and P.B. Harrington, "Detection of Trace Volatile Organic Compounds in Water with a Membrane Interface Ion Mobility Spectrometer," The 52nd Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, New Orleans, LA, March 7, 2001, **2230P**.
- 114) J.M. Perr and P.B. Harrington, "Rapid Screening of Hair Samples using Solid Phase Extraction and Ion Mobility Spectrometry," The 52nd Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, New Orleans, LA, March 8, 2001, **1068**.
- 115) M.L. Patchett and P.B. Harrington, "Detection of Gamma Hydroxybutyrate Using Ion Mobility Spectrometry," The 52nd Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, New Orleans, LA, March 8, 2001, **1067**.
- 116) T.L. Buxton and P.B. Harrington, "Rapid Classification of Bacteria by Ion Mobility Spectrometry," The 52nd Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, New Orleans, LA, March 5, 2001, **384**.
- 117) G. Chen and P.B. Harrington, "Temperature Constrained Radial Basis Function Neural Networks," The 52nd Pittsburgh Conference and Exposition on

Analytical Chemistry & Applied Spectroscopy, New Orleans, LA, March 4, 2001, **312**.

- 118) K.J. Voorhees and P.B. Harrington\*, "Chemometric Opportunities in the Rapid Identification of Bacteria by Mass Spectrometry," The American Society for Mass Spectrometry Sanibel Conference on Informatics and Mass Spectrometry, Sanibel, FL, January 22, 2001.
- 119) P.B. Harrington\*, "Instilling Multivariate Awareness Among Undergraduate Chemistry Students" presented at The 27th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Nashville, TN, September 25, 2000, **414**.
- 120) P.B. Harrington\*, G. Chen, T. Buxton, and A. Urbas, "Real-time Chemometrics" presented at The 27th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Nashville, TN, September 25, 2000, **240**.
- 121) P.B. Harrington\*, T.L. Buxton, G. Chen, P.J. Rauch, and A. Urbas, "Strategies for Smarter Chemical Sensors", 32nd Central Regional Meeting of the American Chemical Society, Covington, KY, May 17, 2000, **020107**.
- 122) M.L. Patchett, J. Perr, and P.B. Harrington, "Characterization of Drugs of Abuse by Ion Mobility Spectrometry and Gas Chromatography-Mass Spectrometry," 32nd Central Regional Meeting of the American Chemical Society, Covington, KY, May 17, 2000, **140211**.
- 123) T. Buxton and P.B. Harrington, "Explosive Detection by Ion Mobility Spectrometry Coupled with Solid Phase Extraction" presented at The 2000 Pittsburgh Conference, New Orleans, LA, March 17, 2000, **1391**.
- 124) A. Urbas and P.B. Harrington, "Instrumental Drift Correction Algorithms for Pattern Recognition of Ion Mobility Spectra" presented at The 2000 Pittsburgh Conference, New Orleans, LA, March 13, 2000, **1712P**.
- 125) G. Chen and P.B. Harrington, "Real-Time Interactive Self-Modeling Mixture Analysis of Ion Mobility Spectra" presented at The 2000 Pittsburgh Conference, New Orleans, LA, March 13, 2000, **41**.
- 126) R. Tucceri, H.H. Richardson and P.B. Harrington, "SIMS Characterization of 3-5 Semiconductors" presented at The 1999 Pittsburgh Conference, Orlando, FL, March 12, 1999, **1474**.
- 127) K.J. Voorhees, M. Xu, F. Basile, P.B. Harrington, A.D. Hendricker, A.J. Madonna, "Advances in *in situ* Thermal Hydrolysis Methylation/MS for the Identification of Microorganisms" presented at The 1999 Pittsburgh



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- 128) S.L. Slagel, P.W. Schmittauer, and P.B. Harrington, "Wireless Data Transmission for Handheld Chemical Sensors" presented at The 1999 Pittsburgh Conference, Orlando, FL, March 9, 1999, **604**.
  - 129) T.L. Buxton, and P.B. Harrington, "Modified Ion Mobility Spectrometer for Enhanced Selectivity" presented at The 1999 Pittsburgh Conference, Orlando, FL, March 9, 1999, **601**.
  - 130) L.A. Shaw and P.B. Harrington, "Analysis of Illegal Drugs by Ion Mobility Spectrometry and SIMPLISMA" presented at The 1999 Pittsburgh Conference, Orlando, FL, March 10, 1999, **2193P**.
  - 131) C. Cai and P.B. Harrington, "Cascade Correlation Neural Networks Using Fourier and Wavelet Compressed Data" presented at The 1999 Pittsburgh Conference, Orlando, FL, March 8, 1999, **249**.
  - 132) C. Wan and P.B. Harrington, "Extracting Features from Artificial Neural Network Models with Sensitivity Analysis" presented at The 1999 Pittsburgh Conference, Orlando, FL, March 8, 1999, **241**.
  - 133) C. Cai and P.B. Harrington, "Prediction of Substructure and Toxicity from Pesticide Mass Spectra" presented at The 25th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Austin, TX, October 15, 1998, **771**.
  - 134) P.B. Harrington\*, "Making the Connection Between Temperature-Constrained Neural Networks and Sensor Measurements" presented at The 25th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Austin, TX, October 15, 1998, **765**.
  - 135) C. Wan and P.B. Harrington, "Determination of Toxic Carbamate Substructures in GC/MS Data with Cascade Correlation Networks" presented at The 25th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Austin, TX, October 15, 1998, 674.
  - 136) D.M. Davis\*, D.B. Shoff, and P.B. Harrington, "Identification of Characteristic IMS Peaks in Forensic Samples" presented at ISIMS '98, Hilton Head, SC, August 12, 1998.
  - 137) P.B. Harrington\*, L. Hu, and C. Cai, "Recovery of Variable Loadings and Eigenvalues Directly from Fourier Compressed Data" presented at ISIMS '98, Hilton Head, SC, August 10, 1998.
  - 138) C. Cai and P.B. Harrington\*, "Linear Discriminant Classification of Fourier and

Wavelet Compressed IMS Data" presented at ISIMS '98, Hilton Head, SC, August 10, 1998.

- 139) J. Stotz and P.B. Harrington, "Accelerant Detection for Arson Investigations Using Ion Mobility Spectrometry" presented at Pittcon '98, New Orleans, LA, March 4, 1998, 884.
- 140) E. Horak and P.B. Harrington, "Calibration and Characterization of a Vapor Generator" presented at Pittcon '98, New Orleans, LA, March 4, 1998, 847.
- 141) C. Wan and P.B. Harrington, "Temperature Constrained Networks for Rapid Screening of Carbamate Compounds in GC-MS Data" presented at Pittcon '98, New Orleans, LA, March 4, 1998, 829.
- 142) C. Cai and P.B. Harrington, "Enhanced Temperature Constrained Cascade Correlation Networks" presented at Pittcon '98, New Orleans, LA, March 2, 1998, 383.
- 143) C. Cai and P.B. Harrington, "Wavelet Compression for Rapid Computation of Large Matrices" presented at The 24th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Providence, RI, October 27, 1997, 619.
- 144) C. Wan, J.Y. Tong, and P.B. Harrington, "A Novel Method for On-site Cocaine Detection with a Hand-held Ion Mobility Spectrometer" presented at The 24th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Providence, RI, October 27, 1997, 102.
- 145) P.B. Harrington\*, "Evaluation of Data and Model Quality" presented at the Optical Society of America Annual Meeting, Long Beach, CA, October 14, 1997.
- 146) P.B. Harrington and C. Wan, "Trace Analysis of Organic Compounds in Water with a Membrane Interfaced Ion Mobility Spectrometer" presented at the 27th International Symposium of Environmental Chemistry, Jekyll Island, GA, June, 1997.
- 147) P.J. Rauch, P.B. Harrington, and D.M. Davis, "Making a Smart Instrument: Chemometric Resolution of Mixture Components by Ion Mobility Clear Down Rates" presented at The 1997 Pittsburgh Conference, Atlanta, GA, March, 228.
- 148) E.S. Reese, D.M. Davis, and P.B. Harrington, "Detection of Diazinon on Apples Using an Ion Mobility Spectrometer" presented at The 1997 Pittsburgh Conference, Atlanta, GA, March, 489.

- 149) C. Wan and P.B. Harrington, "Analysis of Gasoline Contaminated Water with a Membrane Interfaced Ion Mobility Spectrometer" presented at The 1997 Pittsburgh Conference, Atlanta, GA, March, 552P.
- 150) L. Hu, C. Cai, and P.B. Harrington, "Two-Dimensional Fourier Transform Compression of Ion Mobility Spectra" presented at The 1997 Pittsburgh Conference, Atlanta, GA, March, 071.
- 151) C. Cai and P.B. Harrington "Fuzzy Rule-Building Expert Systems Applied to the Rapid Screening of GC/MS Data of Pesticides" presented at The 23rd Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Kansas City, MO, October 1, 1996.
- 152) L. Hu, D.M. Davis, and P.B. Harrington, "Quantitative Analysis of Mixtures by Ion Mobility Spectrometry" presented at The 23rd Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Kansas City, MO, October 1, 1996.
- 153) P.J. Rauch, P.B. Harrington, and D.M. Davis "Near Real Time Implementation of SIMPLISMA for Analysis of IMS Data" presented at The 23rd Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Kansas City, MO, October 1, 1996.
- 154) P.B. Harrington\*, "Chemometric Approaches to Micromachined Analysis" presented at the First OMACC Symposium, Miami University, Oxford, OH, September 5, 1996.
- 155) P.B. Harrington\*, E.S. Reese, L. Hu, P.J. Rauch, and D.M. Davis, "Interactive Self Modeling Mixture Analysis of Ion Mobility Spectra" presented at The Fifth International Symposium on Ion Mobility Spectrometry, Jackson Hole, WY, August 22, 1996.
- 156) P.B. Harrington\*, "Temperature Constrained Cascade Correlation Networks: Evaluation of Interpolation" presented at Proceedings of the Adaptive Parallel Computing Symposium-96, Dayton, OH, August 8-9.
- 157) P.B. Harrington and J.Y. Tong, "Drugs of Abuse Detection with Ion Mobility Spectrometry" presented at The 1996 Pittsburgh Conference, Chicago, IL, March, 894.
- 158) P.R. Rauch, P.B. Harrington, and D.M. Davis, "Food for Thought: Food Freshness Using an Ion Mobility Spectrometer" presented at The 1996 Pittsburgh Conference, Chicago, IL, March, 508.
- 159) E.S. Reese, J.Y. Tong, P.B. Harrington, and D.M. Davis, "Pesticide Detection with Ion Mobility Spectrometry" presented at The 1996 Pittsburgh

Conference, Chicago, IL, March, 484.

- 160) P.B. Harrington, P. Zheng, and D.M. Davis, "Automatic Fourier Transform Deconvolution in Quantitative Analysis of Ion Mobility Spectra" presented at The 1996 Pittsburgh Conference, Chicago, IL, March, 397
- 161) L. Hu, P.B. Harrington and D.M. Davis, "Quantitative Analysis of Ion Mobility Spectra Using Chemometric Data Expansion" presented at The 1996 Pittsburgh Conference, Chicago, IL, March, 395.
- 162) P. Zheng and P.B. Harrington "Quantitative Analysis of Volatile Organic Compounds Using Ion Mobility Spectrometry and Cascade Correlation Networks" presented at The 22nd Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Cincinnati, OH, October 16, 1995.
- 163) P.B. Harrington\*, "Temperature Constrained-Cascade Correlation Neural Networks" presented at The 22nd Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Cincinnati, OH, October 16, 1995.
- 164) P.B. Harrington\*, "Temperature Constrained-Cascade Correlation Neural Networks" presented at the Ohio Aerospace Institute Neural Networks 1995 Symposium, Athens, OH, August 21, 1995.
- 165) P. Zheng\* and P.B. Harrington, "Quantitative Analysis of Volatile Compounds Using Ion Mobility Spectrometry and Cascade Correlation Neural Networks" presented at the Ohio Aerospace Institute Neural Networks 1995 Symposium, Athens, OH, August 21, 1995.
- 166) L. Hu, E. Saulinskas, P. Johnson, and P.B. Harrington, "Evaluation of a Computerized Peptide Sequence Identification System" presented at The 1995 Pittsburgh Conference, New Orleans, LA, March 1995, 890.
- 167) P.B. Harrington and B. Wabuye, "Fuzzy Optimal Associative Memory for Background Prediction of Spectra" presented at The 1995 Pittsburgh Conference, New Orleans, LA, March 1995, 711.
- 168) P.J. Tandler, J.A. Butcher and P.B. Harrington, "Calibration of a Chemometric Detector for Plastic Recycling" presented at The 1995 Pittsburgh Conference, New Orleans, LA, March 1995, 707.
- 169) P.J. Rauch and P.B. Harrington, "Algorithms for Mass Spectral Verification of Chemical Arms Treaties" presented at The 1995 Pittsburgh Conference, New Orleans, LA, March 1995, 550.
- 170) P.B. Harrington and P. Zheng\*, "Making the Connection: Neural Networks and Chemistry" presented at The Dayton Section of the Society of Applied

Spectroscopy October Meeting, Dayton, OH, February 22, 1995.

- 171) P.B. Harrington\*, "Making the Connection: Neural Networks and Chemistry" presented at The Cleveland Section of the American Chemical Society/Society of Applied Spectroscopy October Meeting, Cleveland, OH, October 16, 1994.
- 172) P.B. Harrington\* and P. Zheng, "Quantitative Analysis of Volatile Organic Compounds Using Ion Mobility Spectra and Cascade Correlation Neural Networks" presented at The Third International Workshop on Ion Mobility Spectrometry, Galveston, TX, October, 1994.
- 173) P.B. Harrington, "Evaluation of Cascade Correlation Neural Networks" presented at The 21st Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, St. Louis, MO, October 14, 1994.
- 174) P.J. Tandler, T. Hu, J.A. Butcher, and P.B. Harrington, "A Chemometric Detector for Plastic Recycling" presented at The Fourth Hidden Peak Symposium on Computer-Enhanced Analytical Spectroscopy, Snowbird, UT, June, 1994.
- 175) D.A. Wuersig, B.W. Wabuyeale and P.B. Harrington\*, "Cascade Correlation Neural Networks" presented at the Eastman Kodak Company, Rochester, NY, June 3, 1994.
- 176) D.A. Wuersig and P.B. Harrington\*, "Cascade Correlation Neural Networks" presented at The 11th Annual Quality and Productivity Research Conference, Rochester, NY, June 2, 1994.
- 177) H. Whittenburg, D. King, and P.B. Harrington, "Characterization of Pathogenic Microorganisms Using Pyrolysis High Resolution Gas Chromatography" presented at The 1994 Pittsburgh Conference, Chicago, IL, March 1994, 814.
- 178) D. Wuersig and P.B. Harrington, "Quantitative Spectra-Retention Relationships" presented at The 1994 Pittsburgh Conference, Chicago, IL, March 1994, 792.
- 179) B. Wabuyeale and P.B. Harrington, "A Filter for Spectrochemical Data with an Autoassociative Backpropagation Neural Network" presented at The 1994 Pittsburgh Conference, Chicago, IL, March 1994, 791.
- 180) L. Hu, E. Saulinskas, P. Johnson and P.B. Harrington, "An Intelligent Algorithm for Peptide Sequence Identification" presented at The 1994 Pittsburgh Conference, Chicago, IL, March 1994, 790.
- 181) P. Zheng, D. Davis, and P.B. Harrington, "Comparison of Backpropagation and Counterpropagation Neural Network for Quantitative Analysis of Ion

- Mobility Spectra" presented at The 1994 Pittsburgh Conference, Chicago, IL, March 1994, 641.
- 182) P.B. Harrington, "Optimal Fuzzy Decision Making" presented at The 1994 Pittsburgh Conference, Chicago, IL, March 1994, 640.
  - 183) P.B. Harrington\*, "Spectroscopic Uses of Machine Learning: How to Make Computers Take the Initiative" presented at The Ohio Section of the Society of Applied Spectroscopy, Cincinnati, OH, December 21, 1993.
  - 184) P.B. Harrington\*, "Temperature Constrained Neural Networks: Applications to Quantitative Analysis" presented at The 20th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Detroit, MI, October 19, 1993, 217.
  - 185) P.B. Harrington, "Optimal Fuzzy Decisions for Problems in Analytical Chemistry." presented at the Midwestern University Analytical Chemistry Conference, Indiana University, Bloomington, IN, October 15, 1993.
  - 186) P.B. Harrington\*, "Spectroscopic Uses of Machine Learning: How to Make Computers Take the Initiative." presented at The Indiana Section of the Society for Applied Spectroscopy, Butler University, Indianapolis, IN October 13, 1993.
  - 187) P.B. Harrington\*, "Neural Networks Applied to Analytical Chemistry" presented at the Ohio University  $\Sigma X$  May Meeting, Athens, OH May 1993.
  - 188) J.S. Siegel and P.B. Harrington, "Identification of Hair by Pyrolysis Gas Chromatography" presented at the Regional Undergraduate Chemistry Poster Competition, Lexington, Kentucky, April 1993, 17.
  - 189) P.B. Harrington\*, "Constrained Learning Algorithms for Backpropagation Neural Networks: Local Temperature Maximization: Simulated Annealing Approach" presented at the 205th ACS National Meeting, Denver, CO, March 1993, 32.
  - 190) H. Whittenburg, D. King, B.W. Wabuye and P.B. Harrington, "Characterization of Food Oils Using High Resolution Pyrolysis-Gas Chromatography" presented at the 1993 Pittsburgh Conference, Atlanta, GA, March 1993, 746.
  - 191) B.W. Wabuye and P.B. Harrington, "Applications of Butterfly Neural Networks to Nonlinear Principal Component Analysis" presented at the 1993 Pittsburgh Conference, Atlanta, GA, March 1993, 371.
  - 192) P.J. Tandler and P.B. Harrington, "Optimization of Neural Network

- Configurations by Experimental Design” presented at the 1993 Pittsburgh Conference, Atlanta, GA, March 1993, 369.
- 193) P.B. Harrington, “Constrained Learning Algorithms for Backpropagation Neural Networks: Local Temperature Maximization” presented at the 1993 Pittsburgh Conference, Atlanta, GA, March 1993, 368.
  - 194) P. Zheng and P.B. Harrington, “Cluster Analysis of Secondary Ion Mass Spectra” presented at the 1993 Pittsburgh Conference, Atlanta, GA, March 1993, 039.
  - 195) P.B. Harrington\*, “Minimal Neural Networks: Temperature Jump Training” presented at Federation of Analytical Chemistry and Spectroscopy Societies XIX, Philadelphia, PA, September, 1992.
  - 196) P.J. Tandler and P.B. Harrington, “An Innovative Approach to Classification using Fractal Geometry,” presented at the 1992 Pittsburgh Conference, New Orleans, LA, March, 1992, 376.
  - 197) B. Wabuye and P.B. Harrington, “Applications of Automated Feature Selection Techniques in Quality Evaluation of Food Oils by Infrared Spectroscopy,” presented at the 1992 Pittsburgh Conference, New Orleans, LA, March, 1992, 179.
  - 198) B.W. Pack and P.B. Harrington, “A Novel Network for Multivariate Calibration,” presented at the 1992 Pittsburgh Conference, New Orleans, LA, March, 1992, 175.
  - 199) P.B. Harrington, “Minimal Neural Networks: Concerted Optimization of Multiple Linear Discriminants,” presented at the 1992 Pittsburgh Conference, New Orleans, LA, March, 1992, 174.
  - 200) P.B. Harrington, “Minimal Neural Networks,” presented at the Eastern Analytical Symposium, Somerset, NJ November, 1991.
  - 201) P.B. Harrington, “Applications of Fuzzy Pattern Recognition to Mass Spectrometry,” presented at Federation of Analytical Chemistry and Spectroscopy Societies XVIII, Anaheim, CA, October, 1991.
  - 202) P.B. Harrington\*, “Minimal Neural Networks,” presented at Federation of Analytical Chemistry and Spectroscopy Societies XVIII, Anaheim, CA, October, 1991.
  - 203) P.B. Harrington\*, “Novel Methods of Forensic Identification by Chemical Fingerprints,” The Centennial Symposia of the Ohio Academy of Science, Columbus, OH, April, 1991.

- 204) P.B. Harrington, "Fuzzy Rule-Building Expert System: Minimal Neural Network" presented at the 1991 Pittsburgh Conference, Chicago, IL, March, 1991, 562.
- 205) P.B. Harrington\*, "Digital Distributed Parallel Processing," presented at Federation of Analytical Chemistry and Spectroscopy Societies XVII, Cleveland, OH, October, 1990, 843.
- 206) P.B. Harrington\*, "Fuzzy Rule Building Expert Systems," presented at the Third Hidden Peak Symposium on Computer-Enhanced Analytical Spectroscopy, Snowbird, UT, June, 1990.
- 207) P.B. Harrington, "Comparison of a Neural Network with Rule-Building Expert Systems," presented at the 1990 Pittsburgh Conference, New York, NY, March, 1990, 970.
- 208) P.B. Harrington, S.J. DeLuca, E.W. Sarver, and K.J. Voorhees, "Instrumental Effects on Bacterial Taxonomy by Pyrolysis-Mass Spectrometry," presented at the 1990 Pittsburgh Conference, New York, NY, March, 1990, 1194.
- 209) S.L. DeLuca, E.W. Sarver, P.B. Harrington, and K.J. Voorhees, "Use of Fatty Acids for Identification of Bacteria," presented at U.S. Army CRDEC Conference on Biodetection, Edgewood, MD, November 1989.
- 210) P.B. Harrington, "Rule Building Expert Systems," presented at Midwest Universities Analytical Chemistry Conference, Oxford, OH, October, 1989.
- 211) P.B. Harrington, "Soft Rule Building Algorithms for Multivariate Expert Systems," presented at Federation of Analytical Chemistry and Spectroscopy Societies XVI, Chicago, IL, October, 1989, 664.
- 212) P.B. Harrington\* and K.J. Voorhees, "Rule Building Expert Systems," presented at the 7th Asilomar Conference on Mass Spectrometry, Pacific Grove, CA, September, 1989.
- 213) R.W. Odom, F.R. di Brozolo, P.B. Harrington, and K.J. Voorhees, "Bulk Polymer Analysis Using Laser Ionization Mass Spectrometry and Pattern Recognition Techniques," presented at the 37th ASMS Conference on Mass Spectrometry and Allied Topics, Miami Beach, FL.
- 214) P.B. Harrington and K.J. Voorhees, "Partial Least Squares Applied to Pyrolysis-Mass Spectra of Bacterial Mixtures," presented at the 1989 Pittsburgh Conference, Atlanta, March, 1989, 1529.
- 215) P.B. Harrington and K.J. Voorhees, "MuRES: A Multivariate Expert System," presented at the 1989 Pittsburgh Conference, Atlanta, GA, March, 1989,



1528.

- 216) K.J. Voorhees, P.B. Harrington, T.E. Street, S. Hoffman, S.L. Durfee, J.E. Bonelli and C.S. Firnhaber, "Approaches to Pyrolysis Mass Spectrometry Data Analysis of Biological Materials," presented at the 2nd Hidden Peak Symposium on Computer-Enhanced Analytical Spectroscopy, Snowbird, UT, June, 1988.
- 217) R.W. Odom, F. Radicati di Brozolo, P.B. Harrington, K.J. Voorhees, "Organic Polymer Analysis by Laser Ionization Mass Spectrometry," presented at the 36th ASMS Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, June, 1988.
- 218) J. Bonelli, M. Fairfax, L. Heifets, L. Fink, K.J. Voorhees and P.B. Harrington, "Speciation of Mycobacteria by Curie-Point Pyrolysis," presented at the Academy of Clinical Laboratory Physicians and Scientists, Cincinnati, OH, June, 1988.
- 219) P.B. Harrington and K.J. Voorhees, "A Rule-Building Expert System for the Classification of Pyrolysis-Mass Spectra," presented at the 1988 Pittsburgh Conference, New Orleans, March, 1988, 948.
- 220) P.B. Harrington and T.L. Isenhour, "Expert Strategies for the Temporal Optimization of Robotic Procedures," presented at the 1987 Pittsburgh Conference, Atlantic City, March, 1987.
- 221) T.L. Isenhour, W.A. Schlieper, P.B. Harrington and S.E. Eckert, "Computer Generated Robot Control for the Analytical Laboratory," presented at the Eastern Analytical Symposium, 1986.
- 222) J.C. Marshall, P.B. Harrington, W.A. Schlieper and T.L. Isenhour, "Artificial Intelligence and Robot Control," presented at the International Symposium on Laboratory Robotics, Boston, October, 1986.
- 223) P.B. Harrington and T.L. Isenhour, "A Quantitative Measure of the Reliability of Searches of Spectral Libraries," presented at the 1st Hidden Peak Symposium on Computer-Enhanced Analytical Spectroscopy, Snowbird, UT, June, 1986.
- 224) P.B. Harrington and T.L. Isenhour, "An Expert System for Temporal Optimization of Robotic Procedures," presented at the 1986 Pittsburgh Conference, Atlantic City, March, 1986.
- 225) P.B. Harrington and T.L. Isenhour, "Evaluation of a Multiple Purpose Factor Combined IR/MS Library," presented at the 1985 Pittsburgh Conference, New Orleans, February 1985.