

Curriculum Vitae-23-Sep-08
Peter de Boves Harrington

Address: Center for Intelligent Chemical Instrumentation
Department of Chemistry and Biochemistry
Clippinger Laboratories
Ohio University
Athens, Ohio, USA 45701-2979

Phone: 01-740-994-0265 (Office)
01-740-593-0148 (FAX)

E-mail: Peter.Harrington@Ohio.edu
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

Chercheur Etranger, Université Paul Cézanne, Marseille, FR September-Decemberm
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-Present
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
Dual Level:	Chemical Separation Methods Chemical Separation Methods Lab Spectrochemical Analysis Spectrochemical Analysis Lab Forensic Chemistry
Undergraduate Level:	Quantitative Analysis Quantitative Analysis Lab Fundamentals of Chemistry III

Research Group

Yao Lu	(Ph.D. 2009)
Weiyang Lu	(Ph.D. 2011)
Xiaobo Sun	(Ph.D. 2011)
Zhanfeng Xu	(Ph.D. 2011)

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 Meuller	(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

- 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)₆ 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

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 (12/Sep/2000-15/Dec/2000).

Awards and Recognition

International Journal of Spectroscopy (Editor, 2008-).

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, Liaoning, 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-)

Talanta (Editorial Advisory Board, 2005)

Analytical Sciences Digital Library (Contributing Editor 2003-2005)

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

Peer Review Participation

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, 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 *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 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
Journal of Analytical and Applied Pyrolysis
Journal of the American Society of Mass Spectrometry
Journal of Chemometrics
Journal of Chemical Education
Mikrochimica Acta
Spectroscopy
Talanta
Vibrational Spectroscopy

Professional Affiliations

American Academy of Forensic Sciences (Criminalistics, 2008)
American Chemical Society
Forensic Science Institute of Ohio
International Chemometrics Society
International Society for Ion Mobility Spectrometry
Steering Committee (2005-2007)
Secretary (2006-2007)
International Forensic Science Consortium
North American Academy of Arts & Sciences Fellow (Lifetime Member)
Society for Applied Spectroscopy

Spectroscopy Society of Pittsburgh
Society for Analytical Chemists of Pittsburgh (Lifetime Member)
Sigma Xi

Scientific Committee

The 3rd Symposium on Computer Applications and Chemometrics in Analytical Chemistry, Lake Balaton, Hungary, July 3-7, 2006.

Program Committee

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

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

The 13th 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

Chemometrics, the 59th Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2007), March 6, 2008, New Orleans, LA.

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

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

Modeling, The 15th International Conference on Ion Mobility Spectrometry, July 25, 2006, Honolulu, HI.

The 3rd 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 57th Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, Orlando, FL, March 13, 2006.

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

Instrumentation, The 13th International Conference on Ion Mobility Spectrometry, Gatlinburg, TN, July 28, 2004.

Ionization and Reactant Ions, The 12th 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 FACSS Conference, Nashville, TN, September 2000. **Organized.**

Computational Methods I, The 1998 FACSS Conference, Austin, TX, October, 1998.
Real World Analysis II, The 1997 FACSS Conference, Providence, RI, October, 1997.

Chemometric Applications Using ICP-AES, ICP-MS, and GC-MS Techniques, The 1996 FACSS 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 FACSS Conference, Cincinnati, OH, October 1995.

Making the Connection: Neural Networks and Chemistry, The 1994 FACSS 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, "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 10th 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 3rd 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

Source: Ohio University Growth Fund

Project Title: Master of Science Program in Forensic Chemistry
Investigator: Peter Harrington
Amount Funded: \$147,358

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

Past

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+Luebbe InfraProver 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)
Publications from OU Projects

- 1) Ping Chen, Yao Lu, and P.B. Harrington*, Application of Linear and Nonlinear Discrete Wavelet Transforms to MALDI-MS Measurements of Bacteria for Classification. *Analytical Chemistry*, [10.1021/ac8004549](https://doi.org/10.1021/ac8004549).
- 2) Ping Chen, Yao Lu, and P.B. Harrington*, Biomarker Profiling and Reproducibility Study of MALDI-MS Measurements of Escherichia coli by Analysis of Variance-Principal Component Analysis. *Analytical Chemistry*, **80:5** (2008) 1474-1481.
- 3) Ping Chen and P.B. Harrington*, Discriminant Analysis of Fused Positive and Negative Ion Mobility Spectra Using Multivariate Self-Modeling Mixture Analysis and Neural Networks. *Applied Spectroscopy*, **62:2** (2008) 133-141.
- 4) R.M. O'Donnell, X. Sun, and P.B. Harrington*, Pharmaceutical Applications of Ion and Differential Mobility Spectrometries. *Trends in Analytical Chemistry*, **27:1** (2008) 44-53.
- 5) P.B. Harrington*, C. Laurent, D.F. Levinson, P. Levitt, and S.P. Markey, Bootstrap Classification and Point-Based Feature Selection from Age-Staged Mouse Cerebellum Tissues of Matrix Assisted Laser Desorption/Ionization Mass Spectra using a Fuzzy Rule-Building Expert System. *Analytica Chimica Acta*, **599** (2007) 219-231.
- 6) Yao Lu and P.B. Harrington*, Forensic Application of Gas Chromatography-Differential Mobility Spectrometry with Two-Way Classification of Ignitable Liquids from Fire Debris. *Analytical Chemistry*, **79:17** (2007) 6752-6759.
- 7) Z.Y. Zhang*, Y.M. Wang, G.Q. Fan, and P.B. Harrington, A comparative study of multilayer perceptron neural networks for the identification of rhubarb samples. *Phytochemical Analysis*, **18** (2007) 109-114.
- 8) P. Rearden and P.B. Harrington*, Fuzzy Rule-Building Expert System Classification of Fuel Using Solid Phase Microextraction Two-Way Gas Chromatography Differential Mobility Spectrometric Data. *Analytical Chemistry*, **79:4** (2007) 1485-1491.
- 9) P.B. Harrington*, Statistical Validation of Classification and Calibration Models Using Bootstrapped Latin Partitions. *Trends in Analytical Chemistry*, **25:11** (2006) 1112-1124.
- 10) F. Wang, Z. Zhang*, X. Cui, P.B. Harrington, Identification of rhubarbs by using NIR spectrometry and temperature-constrained cascade correlation networks. *Talanta*, **70** (2006) 1170-1176.
- 11) X. Cui, Z. Zhang*, X. Yuan, J. Zhang, S. Liu, L. Guo, and P.B. Harrington, Application of Density Functional Theoretic Descriptors to Quantitative Structure Activity Relationships with Temperature Constrained Cascade

- Correlation Network Models of Nitrobenzene Derivatives. *Chemical Research in Chinese Universities*, **22:4** (2006) 439-442.
- 12) Z. Zhang*, H. Zhou, S. Liu, and P.B. Harrington, An Application of Takagi-Sugeno Fuzzy System to the Classification of Cancer Patients Based on the Elemental Contents in Serum Samples. *Chemometrics and Intelligent Laboratory Systems*, **82** (2006) 294-299.
 - 13) P.B. Harrington*, N.E. Vieira, P. Chen, J. Espinoza, J.K. Nien, R. Romero, and A.L. Yergey, Proteomic Analysis of Amniotic Fluids Using Analysis of Variance-Principal Component Analysis and Fuzzy Rule-Building Expert Systems Applied to Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry. *Chemometrics and Intelligent Laboratory Systems*, **82** (2006) 283-293.
 - 14) P. Rearden and P.B. Harrington*, Detection of VOCs Using Gas Chromatography-Differential Mobility Spectrometry (GC-DMS). *LabPlus International*, **20:1** (2006) 20-24
(<http://www.labplusinternational.com/artimg/a20061217243159.PDF>).
 - 15) G.M. Bota and P.B. Harrington*, Direct Detection of Trimethylamine in Meat Food Products Using Ion Mobility Spectrometry. *Talanta*, **68:3** (2006) 629-635.
 - 16) R.V. Fox*, R.D. Ball, P.B. Harrington, H.W. Rollins, and C.M. Wai, Holmium Nitrate Complexation with Tri-n-butyl Phosphate in Supercritical Carbon Dioxide. *Journal of Supercritical Fluids*, **36:2** (2005) 137-144.
 - 17) Z.Y. Zhang*, G. Chen, and P.B. Harrington, Detection of trace organic compounds by using ion mobility spectrometry and SIMPLISMA. *Spectroscopy and Spectral Analysis*, **25:9** (2005) 1530-1533.
 - 18) C. Laurent*, D.F. Levinson, S.A. Schwartz, P.B. Harrington, S.P. Markey, R.M. Caprioli, and P. Levitt, Direct Profiling of the Cerebellum by MALDI MS: A Methodological Study in Postnatal and Adult Mouse. *Journal of Neuroscience Research*, **81:5** (2005) 613-621.
 - 19) Z. Zhang* and P.B. Harrington, Recent Studies on Artificial Neural Networks and Their Application. *Current Topics in Analytical Chemistry*, **5** (2005) 24-41.
 - 20) M.L. Ochoa and P.B. Harrington*, Immunomagnetic Isolation of Enterohemorrhagic *Escherichia coli* O157:H7 from Ground Beef and Identification by Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry and Database Searches. *Analytical Chemistry*, **77** (2005) 5258-5267.
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Presentations

Mentoring

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- 2) P.B. Harrington, "Analytical and Forensic Chemistry at Ohio University", Shanghai Jiao Tong University, Shanghai, PRC, December 16, 2006.
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- 7) P.B. Harrington, "Department of Chemistry and Biochemistry at Ohio University", Shanghai University, Shanghai, PRC, December 13, 2006.
- 8) 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.
- 9) P.B. Harrington, "Experimental Design and Optimization" lecture (1.5 hr) given to an undergraduate class at Universität Leipzig, Leipzig, Germany, July 15, 2004.

- 10) P.B. Harrington, "Ohio University's Graduate Program in Chemistry" presented at the Second Ohio Analytical Chemistry Consortium, Columbus, OH, October 31, 2003.
- 11) P.B. Harrington, "Statistical Experimental Design for Chemists" presented at Ohio University, Athens, OH, April 28, 2003.
- 12) 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, "Chemometric Opportunities in the Discovery of Proteomic Biomarkers via Mass Spectrometry", Peking University, Beijing, PRC, July 4, 2008.
- 2) P.B. Harrington, "Three -ics: Chemometrics, Forensics, and Proteomics", Beijing Institute of Technology, Beijing, PRC, July 1, 2008.
- 3) 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.
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- 5) P.B. Harrington, "Three -ics: Chemometrics, Forensics, and Proteomics", University of Missouri, Columbia, MO, October 19, 2007.
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- 7) P.B. Harrington, "Chemometric Opportunities in the Discovery of Proteomic Biomarkers via Mass Spectrometry", Shanghai University, Shanghai, PRC, September 21, 2007.
- 8) 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.
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- 14) 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.
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- 17) P.B. Harrington, "Chemometric Modeling of Ion Mobility and Mass Spectrometric Data", presented at East Carolina University, Greenville, NC, December 3, 2004.
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- 26) 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.
- 27) 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.
- 28) 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.
- 29) 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.
- 30) 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.
- 31) 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.
- 32) 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.
- 33) 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.

- 34) 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.
- 35) 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.
- 36) 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.
- 37) 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.
- 38) 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.
- 39) 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.
- 40) 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.
- 41) 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.
- 42) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems" presented at the Virginia Commonwealth University, Richmond, VA, January, 20, 1998.
- 43) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems" presented at University of North Carolina, Chapel Hill, NC, February 10, 1997.
- 44) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems" presented at Northern Arizona University, Flagstaff, AZ, November 15, 1996.
- 45) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems" presented at the Arizona State University Department of Chemistry, Tempe, AZ, November 14, 1996.

- 46) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems" presented at the Clemson University Department of Chemistry, Clemson, SC, September 19, 1996.
- 47) P.B. Harrington, "Making the Connection Between Neural Networks and Analytical Chemistry" presented at De Pauw University, Greencastle, IN, March 14, 1996.
- 48) P.B. Harrington, "Making the Connection Between Neural Networks and Mass Spectrometry" presented at University of Wales, Swansea, United Kingdom, August 18, 1995.
- 49) 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.
- 50) P.B. Harrington, "Making the Connection: Neural Networks and Chemistry" presented at John Carrol University, Cleveland, OH, October 26, 1994.
- 51) P.B. Harrington, "Chemometrics: New Approaches to Solving Old Problems" presented at Xavier University, Cincinnati, OH, September 16, 1994.
- 52) 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.
- 53) P.B. Harrington, "New Directions in Analytical Chemistry" guest lecturer in conjunction with the Randolph-Macon Chemistry Department's lecture series, Ashland, November, 1990.
- 54) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Marshall University, Huntington, WV, March 1990.
- 55) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Kent State University, Kent, OH, February 1989.
- 56) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Seton Hall University, East Orange, NJ, March 1990.
- 57) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Ohio University, Athens, OH, March 1989.
- 58) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Auburn University, Auburn, AL, March 1989.

- 59) P.B. Harrington, "Statistical Tests for Analytical Chemists" presented at Utah State University, Logan, UT, March, 1985.
- 60) P.B. Harrington, "Pyrolysis Gas Chromatography" presented at University of North Carolina, Chapel Hill, NC, March, 1984.
- 61) P.B. Harrington, "Flavor Modeling Using Headspace and Pyrolysis Gas Chromatography," presented at Randolph-Macon College, Ashland, November, 1981.
- 62) 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, 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.
- 2) P.B. Harrington, "Bootstrap Methods in MALDI-MS: How to Get Something from Nothing", National Institutes of Health, Bethesda, MD, November 9, 2006.
- 3) 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.
- 4) 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.
- 5) 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.
- 6) 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.
- 7) 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.
- 8) 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.

- 9) 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.
- 10) 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.
- 11) 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.
- 12) 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.
- 13) 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.
- 14) 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.
- 15) 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.
- 16) 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.
- 17) 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.
- 18) 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.

- 19) 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.
- 20) 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.
- 21) 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.
- 22) P.B. Harrington, "Making the Connection Between Neural Networks and Food Analysis" presented at Battelle Columbus, OH, May, 1998.
- 23) P.B. Harrington, "Making the Connection Between Neural Networks and Food Analysis" presented at Nabisco, East Hanover, NJ, May 14, 1996.
- 24) 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.
- 25) 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.
- 26) 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.
- 27) 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.
- 28) P.B. Harrington, "Minimal Neural Networks," presented at Leybold Inficon, 2 Technology Place, East Syracuse, NY, March 1992.
- 29) P.B. Harrington, "Minimal Neural Networks," presented at the National Biscuit Company, East Hanover, NJ November, 1991.
- 30) P.B. Harrington, "Minimal Neural Networks," presented at Dow Chemical's Symposium on Neural Network Awareness, Dow Chemical, Freeport, TX, October 1991.

- 31) 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.
- 32) P.B. Harrington, "Intelligent Peptide Sequencing," presented at Applied Biosystems, Inc., Foster City, CA, February, 1991.
- 33) P.B. Harrington, "Fuzzy Rule-Building Expert Systems," presented at Charles Evans and Assoc., Redwood City, CA, February, 1991.
- 34) P.B. Harrington, "Partial Least Squares Analysis Applied to Property Prediction," presented at Nabisco Brands, Inc. East Hanover, NJ, December, 1989.
- 35) P.B. Harrington, "Survey of Pattern Recognition Methods," presented at Teledyne CME, Santa Clara, CA, December, 1989.
- 36) P.B. Harrington, "Demonstration of Resolve Software," U.S. Army CRDEC Quarterly Review of CBMS program, Edgewood, MD, November, 1989.

Presentations at International Scientific Conferences

(*Denotes invited presentation and underlining the presenter)

- 1) P.B. Harrington, "Development of Nonlinear Modeling Methods for Chemical Agent Detection from Differential Mobility Images", The 17th Annual Conference on Ion Mobility Spectrometry, Ottawa, CA, July 24, 2008.
- 2) 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.
- 3) P.B. Harrington*, "Chemometric Opportunities in Proteomic Biomarker Discovery via Mass Spectrometry", Colloquium Spectroscopicum Internationale XXXV, Xiamen, PRC, September 24, 2007.
- 4) 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.
- 5) 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.
- 6) P.B. Harrington, P. Chen, and A. Yergey, "Theoretical Foundations of Analysis of Variance-Principal Component Analysis", presented at the 10th International Conference on Chemometrics in Analytical Chemistry (CAC-2006), Aguas de Lindòia, Brazil, September 12, 2006.

- 7) P.B. Harrington* and Y. Lu, "Forensic Applications of Chemometrics: Classification of Accelerants from Fire Debris by Gas Chromatography-Differential Mobility Spectrometry (GC-DMS)", presented at the 10th International Conference on Chemometrics in Analytical Chemistry (CAC-2006), Aguas de Lindoia, Brazil, September 12, 2006.
- 8) P.B. Harrington*, "Chemometric Opportunities in Proteomic Biomarker Discovery via Mass Spectrometry", presented at the 3rd Symposium on Computer Applications and Chemometrics in Analytical Chemistry (SCAC-2006), Lake Balaton, Hungary, July 5, 2006.
- 9) 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 3rd Symposium on Computer Applications and Chemometrics in Analytical Chemistry (SCAC-2006), Lake Balaton, Hungary, July 4, 2006.
- 10) P. Reardon and P.B. Harrington, "Multiway Preprocessing of Gas Chromatography Differential Mobility Spectrometry (GC-DMS) Data for Curve Resolution of Jet Fuels", presented at the 14th International Conference on Ion Mobility Spectrometry, Maffliers, France, July 27, 2005.
- 11) 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", presented at the 14th International Conference on Ion Mobility Spectrometry, Maffliers, France, July 25, 2005.
- 12) 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.
- 13) 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.
- 14) 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.
- 15) P.B. Harrington*, M.L. Ochoa, N.E. Vieira, A.L. Yergey, "Chemometric Considerations in Proteomic Analyses by Mass Spectrometry", presented at the Chemometrics and Analytical Chemistry 2004, Lisbon, Portugal,

September 20, 2004.

- 16) P.B. Harrington and Libo Cao, "Modeling Nonlinear Wavelet Compressed Ion Mobility Spectrometry", presented at the 12th International Conference on Ion Mobility Spectrometry, Umeå, Sweden, July 28, 2003.
- 17) P.B. Harrington and Libo Cao, "Tutorial on Modeling and Wavelet Compression for Ion Mobility Spectrometrists", presented at the 12th International Conference on Ion Mobility Spectrometry, Umeå, Sweden, July 28, 2003.
- 18) Z. Zhang*, H. Zhou, S. Liu, and P.B. Harrington, "Classification of Cancer Patients Based on ICP-AES Determinations Using Neural Networks" presented at The 9th Beijing Conference and Exhibition on Instrumental Analysis, Beijing, PRC, 2001.
- 19) 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" presented at The Tenth International Conference on Ion Mobility Spectrometry, Wernigerode, Germany, August 15, 2001.
- 20) P.B. Harrington*, T.L. Buxton, G. Chen, P.J. Rauch, L. Shaw, and A. Urbas, "Strategies for Smarter Chemical Sensors" presented at the 7th International Conference on Chemometrics in Analytical Chemistry, Antwerp, Belgium, October 20, 2000.
- 21) P.B. Harrington, T.L. Buxton, G. Chen, P.J. Rauch, L. Shaw, and A. Urbas, "Chemometric Strategies for Smarter Ion Mobility Spectrometers" presented at The 9th International Symposium on Ion Mobility Spectrometry, Halifax, Canada, August 15, 2000.
- 22) T. Buxton and P.B. Harrington, "Modified Ion Mobility Spectrometer for Enhanced Selectivity" presented at The 26th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Vancouver, BC, Canada, October 28, 1999, **705**.
- 23) P.B. Harrington*, J. Wan, C. Cai, and A. Urbas, "Applications of Neural Networks to Environmental Analysis" presented at The 26th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Vancouver, BC, October 27, 1999, **487**.
- 24) P.B. Harrington* and J. Wan, "Sensitivity Analysis Applied to Artificial Neural Networks: What has my neural network actually learned?" presented at The Eighth International Symposium on Ion Mobility Spectrometry, Buxton, United Kingdom, August 9, 1999.

- 25) P.B. Harrington, "Temperature Constrained-Cascade Correlation Networks" presented at the Fifth Scandinavian Chemometrics Conference, Lahti, Finland, August 26, 1997.
- 26) P.B. Harrington, E.S. Reese, P.J. Rauch, C. Wan, and D.M., Davis, "Chemometric Tools for Advantageous Use of Dynamic IMS Data" presented at The 6th International Symposium on Ion Mobility Spectrometry, Bastei, Germany, August 14, 1997.
- 27) P.B. Harrington* and L. Hu, "Copiosity Principle for 21st Century Chemometricians" presented at Chemometrics in Analytical Chemistry, Tarragona, Spain, June 25, 1996.
- 28) P. Johnson, L. Hu, E Saulinskas, and P.B. Harrington, "An Expert System for Amino Acid Sequence Analysis presented at The XIth International Conference on Methods in Protein Structure Analysis, Annecy, FR, September 3, 1996.
- 29) P.B. Harrington*, P. Zheng, and Dennis Davis, "Automatic Deconvolution-Temperature Constrained Cascade Correlation Neural Networks for Ion Mobility Data Analysis" presented at The 4th International Workshop on Ion Mobility Spectrometry, Cambridge, United Kingdom, August 7, 1995.
- 30) P.B. Harrington*, "Minimal Neural Networks" presented at Compana-1992, Jena, Germany, August 25, 1992.
- 31) P.B. Harrington* and B.W. Pack, "FLIN: Fuzzy Linear Interpolating Network" presented at Chemometrics in Analytical Chemistry-1992, Montreal, Quebec, Canada, July 1992.

Presentations at U.S. Scientific Conferences

(*Denotes invited presentation)

- 1) W. Lu and P.B. Harrington, "Theory and Analytical Applications of the Temperature Constrained Radial Basis Function Neural Networks", the 59th Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), March 7, 2008, **2530-7**.
- 2) 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 59th Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), March 6, 2008, **2200-8**.
- 3) 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 59th Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), March 6, 2008, **1930-3**.

- 4) 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 59th Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), March 5, 2008, **1490-8**.
- 5) 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 59th Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), March 5, 2008, **1440-2**.
- 6) D. Melaragno and P.B. Harrington, "Detection of Liquid and Cocktail Explosives by Ion Mobility Spectrometry", the 59th Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), March 5, 2008, **1170-3**.
- 7) Z. Xu, C.E. Bunker, and P.B. Harrington, "Classification and Prediction of Jet Fuel Properties by Near Infrared Spectroscopy", the 59th Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008), March 4, 2008, **430-5**.
- 8) 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**.
- 9) 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**.
- 10) 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**.
- 11) 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.
- 12) 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.
- 13) 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**.

- 14) 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**.
- 15) 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 59th Annual Meeting, San Antonio, TX, February 24, 2007, **B194**.
- 16) 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 33rd Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Lake Buena Vista, FL, September 27, 2006.
- 17) P.B. Harrington*, “Two-way Multivariate Correlation as an Information Theoretic Tool for Measuring Analytical Orthogonality” presented at The 33rd Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Lake Buena Vista, FL, September 25, 2006.
- 18) 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 15th International Conference on Ion Mobility Spectrometry, Honolulu, HI, July 27, 2006.
- 19) 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.
- 20) 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 54th ASMS Conference on Mass Spectrometry, Seattle, WA, June 26, 2006.
- 21) 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.

- 22) 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.
- 23) P.B. Harrington*, "Ion and Differential Mobility Spectrometries: Portable Tools for Crime Scene Investigations", presented at the 115th Annual Meeting of The Ohio Academy of Science, Dayton, OH, April 22, 2006.
- 24) 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 57th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 16, 2006, **2330-1**.
- 25) 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 57th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 16, 2006, **2100-17**.
- 26) L.N. Kishler and P.B. Harrington, "Sensor Fusion for Detection of Toxic Industrial Chemicals", presented at The 57th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 16, 2006, **2100-9**.
- 27) 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 57th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 14, 2006, **1160-8**.
- 28) P.B. Harrington, Ping Chen, Preshious Rearden, and Yao Lu, "Chemometric Opportunities in Forensic Chemical Analysis", presented at The 57th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 13, 2006, replaced **580-2** & **580-3**.
- 29) 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 57th Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, Orlando, FL, March 13, 2006, **580-1**.
- 30) 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.
- 31) 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.
 - 32) 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.
 - 33) 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**.
 - 34) 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**.
 - 35) 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.
 - 36) 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.
 - 37) 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.
 - 38) P.B. Harrington and P. Chen, “Equilibrium Modeling of Ion Mobility Spectra”, presented at The 13th International Conference on Ion Mobility Spectrometry, Gatlinburg, TN, July 29, 2004.
 - 39) 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 13th International Conference on Ion Mobility Spectrometry, Gatlinburg, TN, July 25, 2004.

- 40) P. Rearden and P.B. Harrington, "Solid Phase Microextraction Ion Mobility Spectrometry for the Selective Detection of Volatile Aldehydes", presented at The 31st Annual Conference of the National Organization of the Professional Advancement of Black Chemists and Chemical Engineers, San Diego, CA, April 13, 2004.
- 41) 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.
- 42) 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.
- 43) 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.
- 44) 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**.
- 45) 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**.
- 46) 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**.
- 47) 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**.

- 48) 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**.
- 49) P.B. Harrington and L. Cao, "Chemometric Modeling of Mass Spectra", presented at the 2nd Ohio Analytical Chemistry Consortium, Columbus, OH, October 31, 2003.
- 50) 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 29th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Ft. Lauderdale, FL, October 21, 2003.
- 51) 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**.
- 52) 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**.
- 53) 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**.
- 54) 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**.
- 55) P.B. Harrington*, "Chemometrics Opportunities in Ion Mobility and Mass Spectrometries" presented at The 1st Ohio Analytical Chemistry Consortium, Columbus, OH, November 8, 2002.
- 56) 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.
- 57) 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 Cr_xO_y^- in an Ion Trap Secondary Ion Mobility Spectrometer" presented at The 1st Ohio Analytical Chemistry Consortium, Columbus, OH, November 8, 2002.

- 58) 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 Cr_xO_y^- in an Ion Trap Secondary Ion Mobility Spectrometer" presented at The 29th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Providence, RI, October 15, 2002, **330**.
- 59) 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^N" presented at the 2002 Chemometrics in Analytical Chemistry Meeting, Seattle, WA September 25, 2002.
- 60) 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.
- 61) P.B. Harrington*, G. Chen, and N.L. Schmitt, "Detection of Biogenic Amines in Foods Using Ion Mobility Spectrometry and Chemometrics" presented at the 224th American Chemical Society National Meeting, Boston, MA, August 20, 2002, **192**.
- 62) A.K. Gianotto, B.D.M. Hodges, A.D. Appelhans, P.B. Harrington, G.S. Groenewold, M. T. Benson, "Oxidation of Cr_xO_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**.
- 63) 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**.
- 64) 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**.
- 65) 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**.
- 66) 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**.

- 67) 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**.
- 68) P.B. Harrington*, T.L. Buxton, and G. Chen, "Chemometric Strategies for Smart Ion Mobility and Mass Spectrometries," The 115th AOAC INTERNATIONAL Annual Meeting, Kansas City, MO, September 11, 2001.
- 69) P.B. Harrington*, A.A. Urbas, K.J. Voorhees, and J. Rees, "Wavelet Compression and De-noising of MALDI-MS Measurements of Bacteria," The 49th American Society for Mass Spectrometry Conference, Chicago, IL, May 31, 2001, **ThOCpm**.
- 70) 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**.
- 71) 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**.
- 72) 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**.
- 73) 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**.
- 74) 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**.
- 75) 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.

- 76) 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**.
- 77) 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**.
- 78) 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**.
- 79) 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**.
- 80) 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**.
- 81) 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**.
- 82) 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**.
- 83) 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**.
- 84) 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 Conference, Orlando, FL, March 11, 1999, **1292**.
- 85) 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**.
- 86) 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**.

- 87) 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**.
- 88) 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**.
- 89) 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**.
- 90) 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**.
- 91) 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**.
- 92) 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.
- 93) 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.
- 94) 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.
- 95) 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.
- 96) 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.
- 97) E. Horak and P.B. Harrington, "Calibration and Characterization of a Vapor Generator" presented at Pittcon '98, New Orleans, LA, March 4, 1998, 847.
- 98) 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.
- 99) C. Cai and P.B. Harrington, "Enhanced Temperature Constrained Cascade Correlation Networks" presented at Pittcon '98, New Orleans, LA, March 2, 1998, 383.
 - 100) 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.
 - 101) 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.
 - 102) P.B. Harrington*, "Evaluation of Data and Model Quality" presented at the Optical Society of America Annual Meeting, Long Beach, CA, October 14, 1997.
 - 103) 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.
 - 104) 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.
 - 105) 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.
 - 106) 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.
 - 107) 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.
 - 108) 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.

- 109) 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.
- 110) 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.
- 111) P.B. Harrington*, "Chemometric Approaches to Micromachined Analysis" presented at the First OMACC Symposium, Miami University, Oxford, OH, September 5, 1996.
- 112) 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.
- 113) 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.
- 114) 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.
- 115) 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.
- 116) 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.
- 117) 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
- 118) 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.
- 119) 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.

- 120) 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.
- 121) P.B. Harrington*, "Temperature Constrained-Cascade Correlation Neural Networks" presented at the Ohio Aerospace Institute Neural Networks 1995 Symposium, Athens, OH, August 21, 1995.
- 122) 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.
- 123) 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.
- 124) 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.
- 125) 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.
- 126) 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.
- 127) 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.
- 128) 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.
- 129) 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.
- 130) 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.
- 131) 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.
- 132) D.A. Wuersig, B.W. Wabuyele and P.B. Harrington*, “Cascade Correlation Neural Networks” presented at the Eastman Kodak Company, Rochester, NY, June 3, 1994.
 - 133) 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.
 - 134) 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.
 - 135) D. Wuersig and P.B. Harrington, “Quantitative Spectra-Retention Relationships” presented at The 1994 Pittsburgh Conference, Chicago, IL, March 1994, 792.
 - 136) B. Wabuyele 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.
 - 137) 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.
 - 138) 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.
 - 139) P.B. Harrington, “Optimal Fuzzy Decision Making” presented at The 1994 Pittsburgh Conference, Chicago, IL, March 1994, 640.
 - 140) 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.
 - 141) 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.
 - 142) 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.
- 143) 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.
 - 144) P.B. Harrington*, "Neural Networks Applied to Analytical Chemistry" presented at the Ohio University ΣX May Meeting, Athens, OH May 1993.
 - 145) 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.
 - 146) 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.
 - 147) 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.
 - 148) 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.
 - 149) 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.
 - 150) P.B. Harrington, "Constrained Learning Algorithms for Backpropagation Neural Networks: Local Temperature Maximization" presented at the 1993 Pittsburgh Conference, Atlanta, GA, March 1993, 368.
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