# Curriculum Vitae (9/4/2020)



## Peter de Boves Harrington

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## Education

PhD    (Analytical Chemistry), University of North Carolina, Chapel Hill, NC, 1988
       Dissertation Advisor, Thomas L. Isenhour
       Dissertation, "Applications of Pattern Recognition and Artificial Intelligence to Some Problems in Analytical Chemistry"

BS     (Chemistry), Randolph-Macon College, Ashland, VA, 1980

## Professional Experience

Chemistry Mapping, Inc., Board of Directors, 2017-2018
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,

2002-2019
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 Chemistry 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**

| | |
|---|---|
| Gobind Sah | (PhD, 2024) |
| Qudus Ayodeji Thanni | (PhD, 2024) |
| Zewei Chen | (PhD, 2020) |
| Yifei Wang | (Research Assistant Professor, 2018) |
| Ping Geng | (Research Associate Professor, 2019) |
| Jianghao Sun | (Research Associate Professor, 2019) |

**Thesis**

**BS**

Amanda McKeon, "Differentiation of Ignitable Liquids in Fire Debris Using Solid-Phase Microextraction Paired with Gas Chromatography-Mass Spectroscopy and Chemometric Analysis", (BS 2019).

Maryssa Beasley, "Obtaining Unique Fingerprints from Human Hair Samples Using Proteomic Data", (BS 2017).

Anne Marie Esposito, "Detection of Cocaine and its Interferents by Ion Mobility Spectrometry coupled with SIMPLSMA and ALS", (BS 2017).

**MS**

Katie Kohoutek, "Electrospray Ionization Ion Mobility Mass Spectrometry" (MS 2020).

Alessandra Paul, "Chemometric Applications in the Mass Spectrometric Studies of the Metabolome" (MS 2020).

Yue Tang, "Non-Integer Root Transformations for Preprocessing Nano-Electrospray Ionization High Resolution Mass Spectra for the Classification of Cannabis" (MS 2018).

Xue Zhao, "Determination of 1,8 Cineole in Fresh Rosemary and Sage Leaves by Solid-phase Microextraction and Gas Chromatography/Mass Spectrometry" (MS 2017).

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).

**Dissertation**

**PhD**

Ahmet K. Aloglu, "Characterization of Foods by Chromatographic and Spectroscopic Methods Coupled to Chemometrics", (PhD 2018).

Xinyi Wang, "Characterization of Botanicals by Nuclear Magnetic Spectroscopy and Mass Spectrometry Chemical Profiling", (PhD 2018).

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).

Weiying 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 $Mo(CO)_6$ 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 Wabuyele "Application of Associative Memories for Background
Correction of Spectra" (PhD 1995).

**Visiting Scholars**

Baojun Ding, "Support Vector Elastic Nets", Dalian University of Technology,
Dailian, PRC, (15/Oct/2019-15/Mar/2020).

Alfred Christy, "Near Infrared Spectroscopy of Cements", Agder University College,
Kristiansand, Norway, (01/Mar/2019-31/Jul/2019).

Hamid Abdollahi, "Chemometric Theory", Institute for Advanced Studies in Basic
Sciences, Zanjan, Iran, (20/Jun/2018-31/Aug/2018).

Xiaofei Wang, "Detection of Opioids by Mass Spectrometry", Forensic Science
Division in Forensic Science Division of the Public Security Department of
Liaoning Province, China, (1/Jan/2018-31/Dec/2019).

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**

*AOAC-Int* Editorial Advisory Board 2020

*Society for Applied Spectroscopy Fellow Award 2020*

*OHIO President's Research Scholar 2019*

*Finalist SciX 2019 Innovation Award*

*EAS Award for Outstanding Achievement in Chemometrics* 2019

*Advances in Chemical Research* (Editorial Advisory Board, 2018-)

*Molecules* (Editorial Advisory Board, 2018-)

*Analytics* (Editorial Advisory Board, 2017-)

*Investigative Forensic Sciences* (Editor, 2016-2018)

*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, Washington DC, June 18-19, 2018 (7).
      R&D in Forensic Science for Criminal Justice Purposes, Standing Review Panel
      Impression and Trace Evidence, Arlington, VA, June 13-14, 2016 (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 16-17, 2014 (4).

National Science Foundation
      National Science Foundation, CMI Virtual, April 4-5, 2019 (6)
      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, 2019)
AOAC-Int (2020-)

The Coblentz Society (2019)
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
      Governing Board (2019-2022)
      Publications Committee (2019-2022)

Sigma Xi **Secretary** (2012-2019)
      Local Section Ohio University, Athens, OH
Sigma Xi **President** (2005-2012)
      Local Section Ohio University, Athens, OH

**Scientific Committee**
*Chemometrics in Analytical Chemistry* 2020, 21-26 June 2020, Courmayeur, Italy.

*International Academic Committee*, Advances in Pharmaceutical Analysis 2017, November 17-19, 2017, Wuhan, PRC.

The 16th Chemometrics in Analytical Chemistry, Barcelona, Spain, June 6-10, 2016.

The 15th Chemometrics in Analytical Chemistry, Changsha, China, June 22-26, 2015.

The 2nd International Symposium on Profiling 2015 (ISPROF-2015), Caparica, Portugal, September 21-24, 2015.

The 1st International Symposium on Profiling 2013 (ISPROF-2013), Caparica, Portugal, September 2-4, 2013.

The 3rd 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 2020, October 11-16, 2020, Sparks, NV.

*Chemometrics Section Chair,* The Federation of Analytical Chemistry and Spectroscopy Societies, SciX 2019, October 13-18, 2019, Palm Springs, CA.

*Chemometrics Section Chair,* The Federation of Analytical Chemistry and Spectroscopy Societies, SciX 2018, October 21-26, 2018, Atlanta, GA.

2nd World Congress on Pharmaceutical and Chemical Sciences, July 23-25, 2018, Bologna, Italy.  **Program Chair**

9th Edition of International Conference on Analytical Chemistry, Analytical Chemistry 2018, March 26-28, 2018, Vienna, Austria.  **Program Chair**

70th Midwestern Universities Analytical Chemistry Conference, MUACC 2017, October 19-21, 2017, Athens, OH.

*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 2nd International Symposium on Profiling 2015 (ISPROF-2015), Caparica, Portugal, September 21-23, 2015, Scientific Committee.

The 1st 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 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**
*Artificial Intelligence in Pharma,* The Federation of Analytical Chemistry and
Spectroscopy Societies SciX 2018, October 16, 2019, Palm Springs, CA, **co**-**Organized**.

*New Frontiers in Chemometrics,* The Federation of Analytical Chemistry and
Spectroscopy Societies SciX 2018, October 25, 2018, Atlanta, GA, **Organized**.

*Opening Session and Keynote Session*, 2nd World Congress on
PHARMACEUTICAL AND CHEMICAL SCIENCES, July 23-25, 2018, Bologna, Italy.
**Program Chair and Presider**

*Opening Session and Keynote Session*, 9th Edition of International Conference on
Analytical Chemistry, Analytical Chemistry 2018, March 26-28, 2018, Vienna,
Austria. **Program Chair and Presider**

*Final Session*, Advances in Pharmaceutical Analysis 2017, November 17-19, 2017,
Wuhan, PRC.

*Multiblock Methods: The key to measurement fusion,* The Federation of Analytical
Chemistry and Spectroscopy Societies SciX 2017, October 13, 2017, Reno, NV, **Co-Organized**.

*New Frontiers in Chemometrics,* The Federation of Analytical Chemistry and
Spectroscopy Societies SciX 2017, October 10, 2017, Reno, NV, **Organized**.

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

*Chemometrics,* 5th 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 67th American Academy of Forensic Sciences Annual Meeting, February 19, 2015, Orlando, FL.

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

*Final Session*, The 1st 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 59th Annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2008)*, 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 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*, "The End of Science, Big Data, and the Rise of Machine Intelligence", Federation of Analytical Chemistry and Spectroscopy Societies SciX 2018, Atlanta, GA, October 26, 2018.

P.B. Harrington*, "Cascading and Enhanced Restricted Boltzmann Machines for Feature Expansion of Spectra", Chemometrics in Analytical Chemistry (CAC 2018), Halifax, Canada, June 27, 2018.

P.B. Harrington, "Application of Restricted Boltzmann Machines to Analytical Chemistry", Chemometrics in Analytical Chemistry 2018, Vienna, Austria, March 25-28.

P.B. Harrington, "Enhanced Restricted Boltzmann Machines for Classification of Analytical Measurements", WSC-11, St Petersburg, Russia, February 27, 2018.

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 1st 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 6th 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 the10th 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 the3rd 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: ARS Post Doctorate
Investigator:  Peter Harrington
Amount Funded: $400,000
Period:  7/1/2019-09/30/2020

Source: Houston Forensic Science Center
Project Title: Probability Measures of Mass Spectral Library Search Results
Investigator: Peter Harrington
Amount Funded: $108,021
Period: 7/1/2019-12/31/2019

Source:  National Science Foundation
Project Title: EAGER: Development of Statistically Significant Reaction Models
        Describing Electrochemical Conversion of Biomass
Investigator:  John Staser

Amount Funded: 149,842
Period: 8/27/2019-7/31/2021

**Past**
Source:  US Department of Agriculture
Project Title: ARS Post Doctorate
Investigator:  Peter Harrington
Amount Funded: $324,624
Period:  9/1/2019-09/30/2020

Source:  US Department of Agriculture
Project Title: ARS Post Doctorate
Investigator:  Peter Harrington
Amount Funded: $117,903
Period:  7/1/2018-06/30/2019

Source: Department of Energy
Project Title:  Biomass Electrochemical Reactor for Upgrading Biorefinery Waste to
        Industrial Chemicals and Hydrogen
Investigator: John Staser
Amount Funded: $1,472,724
Period: 3/1/2016-2/28/2019

Source:  US Department of Agriculture
Project Title: ARS Post Doctorate
Investigator:  Peter Harrington
Amount Funded: $103,212
Period:  9/1/2018-08/31/2019

Source:  US Department of Agriculture
Project Title: ARS Post Doctorate
Investigator:  Peter Harrington
Amount Funded: $70,000
Period:  1/1/2015-08/31/2019

Source:  US Department of Agriculture
Project Title: ARS Post Doctorate
Investigator:  Peter Harrington
Amount Funded: $90,450
Period:  10/1/2017-09/30/2018

Source:  US Department of Agriculture
Project Title:  ARS Post Doctorate
Investigator:  Peter Harrington
Amount Funded: $33,501

Period:  1/1/2016-8/31/2017

Source:  US Department of Agriculture
Project Title:  ARS Post Doctorate
Investigator:  Peter Harrington
Amount Funded: $73,499
Period:  1/1/2015-8/31/2018

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: 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

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:  $29,998
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:  $59.989
Period:  5/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:  INSSI
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) A. Paul and P.B. Harrington*, Chemometric Applications in Metabolomic

Studies Using Chromatography-Mass Spectrometry submitted to Trends in Analytical Chemistry, TrAC.

2) Y. Wang, P.B. Harrington, and P. Chen*, "Metabolomic profiling and comparison of major cinnamon species using UHPLC–HRMS", in press at *Analytical and Bioanalytical Chemistry.*

3) P.B. Harrington, Limits of Detection Revisited submitted to *Talanta*.

4) L. Wang*, R. Yang; L. Qu, and P.B. Harrington, Electrostatic repulsion strategy for high-sensitive and selective determination of dopamine in presence of uric acid and ascorbic acid submitted to *Talanta.*

5) J. Du, R. Yang*, H. Mao, J. Li, L. Qu*, and 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 *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*.

6) Y. Zhou, R. Yang*, Y.P. Pu, J. Li, L. Qu*, and P.B. Harrington, An ultrasensitive spectrophotometry sensor for tartrazine detection based on poly (diallyldimethylammonium chloride) modified nano-silver submitted to *Sensors & Actuators: B. Chemical*.

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

1) Y. Wang, P.B. Harrington, and P. Chen*, Quantitative analysis of proanthocyanidins in cocoa using cysteamine induced thiolysis and reversed-phase UPLC. *Analytical and Bioanalytical Chemistry* (2020) DOI: 10.1007/s00216-020-02669-7.

2) Y. Wang, P.B. Harrington, T. Chang, X. Wu, and P. Chen*, Analysis of Cranberry Proanthocyanidins Using UPLC - Ion mobility - High Resolution Mass spectrometry.  *Analytical and Bioanalytical Chemistry* (2020) DOI: 10.1007/s00216-020-02601-z.

3) Z. Chen, M. NaderiNasrabadi, J.A. Staser, and P.B. Harrington*, Generalized Standard Addition Method to Characterize an Electrolytic Lignin Reactor using Ultraviolet Spectroscopy.  *Journal of Analysis and Testing* (2020) DOI: 10.1007/s41664-020-00119-y.

4) Z. Yuan, L. Zhang*, D. Wan, J. Mao, J. Jiang, Q. Zhang, P.B. Harrington, and P. Li, Detection of flaxseed oil multiple adulteration by near-infrared spectroscopy and nonlinear one class partial least squares discriminant analysis. *LWT-Food Science and Technology* (2020) DOI:

10.1016/j.lwt.2020.109247.

5)  P.B. Harrington*, Enhanced Zippy Restricted Boltzmann Machine for Feature Extraction and Classification Enhancement of Analytical Data. *Journal of Chemometrics* (2020) DOI: 10.1002/cem.3228.

6)  L. Wang, R. Yang*, L. Qu, and P.B. Harrington, Electrostatic repulsion strategy for high-sensitive and selective determination of dopamine in the presence of uric acid and ascorbic acid. *Talanta* (2019) DOI: 10.1016/j.talanta.2019.120626.

7)  Y. Wang, P.B. Harrington, and P. Chen*, Analysis of phenolic compositions in cranberry dietary supplements using UHPLC-HRMS. *Journal of Food Composition and Analysis* (2019) **86** DOI:   10.1016/j.jfca.2019.103362.

8)  Z. Chen and P.B. Harrington*, Pipeline for High-Throughput Modeling of Marijuana and Hemp Extracts.  *Analytical Chemistry* (2019) **91(22)** 14489-14497 DOI:   10.1021/acs.analchem.9b03290.

9)  J.D. McChesney*, J. Dou, P.B. and Harrington, The Development of Botanical Drugs – A Review. *Pharmaceutical Regulatory Affairs* (2019) **8(2)** 1-9 ISSN: 2167-7689.

10)  Z. Chen and P.B. Harrington*, Automatic Soft Independent Modeling for Class Analogies. *Analytica Chimica Acta* (2019) DOI: https://doi.org/10.1016/j.aca.2019.09.035.

11)  M. NaderiNasrabadi, F. Bateni, Z. Chen, P.B. Harrington, and J.A. Staser*, Biomass-depolarized Electrolysis. *Journal of the Electrochemical Society* (2019) **166(10)** E317-E322 DOI: 0.1149/2.1471910jes.

12)  L. Wang, R. Yang, Ji. Li, L. Qu*, and P.B. Harrington, A highly selective and sensitive electrochemical sensor for tryptophan based on the excellent surface adsorption and electrochemical properties of PSS functionalized graphene. *Talanta* (2018) **196** 309-316 DOI: 10.1016/j.talanta.2018.12.058.

13)  Y. Tang and P.B. Harrington*, Non-Integer Root Transformations for Preprocessing Nano-Electrospray Ionization High-Resolution Mass Spectra for the Classification of Cannabis. *Analytical Chemistry* (2018) **91(2)** 1328-1334 DOI: 10.1021/acs.analchem.8b03145.

14)  Z. Chen, P.B. Harrington*, and S.F. Baugh, High-throughput Authentication of *Cannabis* and Hemp Extracts Using an Ultraviolet Microplate Reader and Multivariate Classifiers.  *Journal of Analysis and Testing* (2018) **2(3)** 210-222 DOI: 10.1007/s41664-018-0075-3.

15) Y. Wang, N. Vorsa, P.B. Harrington, and P. Chen*, Non-Targeted Metabolomic Study on Variation of Phenolics in Different Cranberry Cultivars Using UPLC-IM-HRMS. *Journal of Agricultural and Food Chemistry* (2018) **66(46)** 12206–12216 DOI: 10.1021/acs.jafc.8b05029.

16) M. Jie, S. Yu, F. Yu, L. Liu, L. He, Y. Li, H. Zhang, and L. Qu*, P.B. Harrington, and Y. Wu, A ultrasensitive chemiluminescence immunoassay for fumonisin B1 detection in cereals based on gold-coated magnetic nanoparticles. *Journal of the Science of Food and Agriculture*. (2018) **98** 3384-3390 DOI: 10.1002/jsfa.8849.

17) X. Wang and P.B. Harrington*, Differentiating Rice Varieties by Inductively Coupled Plasma Mass Spectrometry Chemical Profiling with Singular Value Decomposition Background Correction, *Journal of Analysis and Testing*. (2018) **2** 138-148 DOI:  10.1007/s41664-018-0055-7.

18) P.B. Harrington*, Feature Expansion by a Continuous Restricted Boltzmann Machine for Near-Infrared Spectrometric Calibration, *Analytica Chimica Acta*. (2018) **1010** 20-28 DOI:  10.1016/j.aca.2018.01.026.

19) X. Wang, P.B. Harrington*, and S.F. Baugh, Effect of Preprocessing High-Resolution Mass Spectra on the Pattern Recognition of Cannabis, Hemp, and Liquor, *Talanta* (2018) **180** 229-238 DOI:  10.1016/j.talanta.2017.12.032.

20) P. Liu, X. Zhang, B. Pan, Mi. Wei, Z. Zhang*, P.B. Harrington, Classification of Sand Grains by Terahertz Time-Domain Spectroscopy and Chemometrics. *International Journal of Environmental Research* (2018) **13(1)** 143-160 DOI: 10.1007/s41742-018-0159-y.

21) P.B. Harrington, Multiple Versus Single Set Validation to Avoid Mistakes, *CRC Critical Reviews in Analytical Chemistry.*  (2018) **48(1)** 33-46 DOI: 10.1080/10408347.2017.1361314.

22) A.K. Aloglu and P.B. Harrington*, Differentiation of Bovine, Porcine, and Fish Gelatins by Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIRS) Coupled with Pattern Recognition. *Journal of Food Composition and Analysis*.  (2018) **101(1)** 221-226 DOI: 10.5740/jaoacint.17-0244.

23) J. Wang, Z. Zhang*, Y. Yang, Y. Xiang, and P.B. Harrington, Identification of Rhubarb Samples by Terahertz Time-Domain Spectroscopy Combined with Principal Component Analysis-Linear Discriminant Analysis and Support Vector Machine, *Spectroscopy and Spectral Analysis.*  (2017) **37(5)** 1606-1611 ISSN: 1000-0693 (2017) 05-1606-06.

24) 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. *Journal of Research Analytica* (2017) **3(3)** 91-95 ISSN: 2473-2230.

25) X. Wang, P.B. Harrington*, and S.F. Baugh, Comparative Study of NMR Spectral Profiling for the Characterization and Authentication of *Cannabis*, *Journal of AOAC-Int*. (2017) **100(5)** 1356-1364 DOI:  10.5740/jaoacint.17-0089.

26) 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.

27) 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.

28) 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** 1-11 DOI: 10.1007/s41664-017-0003-y.

29) P.B. Harrington*, Automated Support Vector Regression, *Journal of Chemometrics* (2017) **31** 1-14 DOI:  10.1002/cem.2867.

30) 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.

31) 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.

32) N.R. Saichek, C.R Cox, S. Kim, P.B. Harrington, N.R. Stambach, and K. Voorhees*, Strain-level *Staphylococcus* differentiation by $CeO_2$-metal oxide laser ionization mass spectrometry fatty acid profiling.  *BMC Microbiology* (2016) **16:72** 1-11 DOI:  10.1186/s12866-016-0658-y.

33) 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.

34) 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.

35) 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.

36) 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.

37) P.B. Harrington*, Support Vector Machine Classification Trees.  *Analytical Chemistry* (2015) **87:21** 11065-11071 DOI: 10.1021/acs.analchem.5b03113.

38) 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.

39) 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.

40) 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.

41) 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.

42) M. Zhang, Y. Zhao, P.B. Harrington, and Pei Chen*, Differentiation of *Aurantii*

*Fructus Immaturus* and *Fructus Poniciri Trifoliatae Immaturus* by Flow-injection with Ultraviolet Spectroscopic Detection and Proton Nuclear Magnetic Resonance using Partial Least-squares Discriminant Analysis. *Analytical Letters* (2015) DOI: 10.1080/00032719.2015.1045588.

43) 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.

44) 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.

45) 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.

46) 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.

47) 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.

48) 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.

49) 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.

50) 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.

51) 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.

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**Presentations**
**Mentoring**
1)  P.B. Harrington*, "Speed Mentoring", The Eastern Analytical Symposium, Princeton, NJ, November 18, 2019.

2)  P.B. Harrington, "The Art of Writing Scientific Research Papers", Zhengzhou University, Zhengzhou, PRC, May 25, 2016.

3)  P.B. Harrington, "Introduction to Chemometrics", The Colorado School of Mines, Golden, CO, November 8, 2010.

4)  P.B. Harrington, "Chemistry Opportunities at OHIO University", Beijing Institute of Technology, Beijing, PRC, July 1, 2008.

5)  P.B. Harrington, "Analytical and Forensic Chemistry at Ohio University", Shanghai Jiao Tong University, Shanghai, PRC, December 16, 2006.

6)  P.B. Harrington, "Department of Chemistry and Biochemistry at Ohio University", Shanghai Jiao Tong University, Shanghai, PRC, December 16, 2006.

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10)  P.B. Harrington, "Department of Chemistry and Biochemistry at Ohio University", Shanghai University, Shanghai, PRC, December 13, 2006.

11)  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.

12)  P.B. Harrington, "Experimental Design and Optimization" lecture (1.5 hr)

given to an undergraduate class at Universität Leipzig, Leipzig, Germany, July 15, 2004.

13) P.B. Harrington, "Ohio University's Graduate Program in Chemistry" presented at the Second Ohio Analytical Chemistry Consortium, Columbus, OH, October 31, 2003.

14) P.B. Harrington, "Statistical Experimental Design for Chemists" presented at Ohio University, Athens, OH, April 28, 2003.

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**Invited Scientific Presentations at Universities and Colleges**
  1) P.B. Harrington, "AI, the End of Science, and the Enhanced Zippy Restricted Boltzmann Machine (EZRBM)", University College Dublin, Dublin, Ireland, May 21, 2019.

  2) P.B. Harrington, "A Robust Restricted Boltzmann Machine for Small Spectral Datasets" in Dynamical Systems and Mathematical Biology Seminar, Ohio University, Athens, OH, October 16, 2018.

  3) P.B. Harrington, "High-throughput Chemotyping of Botanical Products Using Spectroscopy", Aix-Marseille Université, Marseille, France, July 27, 2018.

  4) P.B. Harrington and Y. Tang, "Adventures in Chemometrics:  Optimization of Experiments to Artificial Intelligence", Shandong Normal University, Jinan, PRC, May 19, 2018.

  5) P.B. Harrington, "Chemometric Opportunities in Metabolomics", University of Louisville, Louisville, KY, September 15, 2017.

  6) P.B. Harrington, "Bootstrapping as a Tool to Automate Chemometric Methods", Capital Normal University, Beijing, China, May 10, 2017.

  7) P.B. Harrington, "Chemometric Tools for the Characterization of Complex Materials", Tsinghua University, Beijing, China, May 9, 2017.

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March 21, 2017.

10) P.B. Harrington, "Application of Support Vector Machine Classification Trees to the Authentication of Traditional Chinese Medicines", Zhengzhou University, Zhengzhou, PRC, May 25, 2016.

11) 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.

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13) 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.

14) 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.

15) P.B. Harrington, "Chemometric Opportunities for Forensic Chemical Analysis", Department of Photochemistry, Bowling Green State University, Bowling Green, OH, December 8, 2014.

16) 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.

17) 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.

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19) P.B. Harrington, "Fuzzy Optimal Associative Memories for the Authentication of Nutraceuticals by Mass Spectrometry", Shanghai University, Shanghai, PRC, October 15, 2012.

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31) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", The Colorado School of Mines, Golden, CO, November 9, 2010.

32) P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Universitetet i Bergen, Bergen, NO, August 31, 2010.

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64) P.B. Harrington, "Chemometric Modeling of Ion Mobility and Mass Spectrometric Data", presented at East Carolina University, Greenville, NC, December 3, 2004.

65) 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.

66) 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.

67) P.B. Harrington, "Chemometrics: New Tools for Solving Old Problems in Ion Mobility Spectrometries" presented at Universität Leipzig, Leipzig, Germany, July 15, 2004.

68) P.B. Harrington, "Forensic Adventures with Ion Mobility and Mass Spectrometries" presented at Ohio Wesleyan University, Delaware, OH, March 19, 2004.

69) 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.

70) 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.

71) 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.

72) 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.

73) 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.

74) 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.

75) 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.

76) 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.

77) 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.

78) 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.

79) 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.

80) 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.

81) 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.

82) 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.

83) 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.

84) 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.

85) 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.

86) 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.

87) 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.

88) 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.

89) P.B. Harrington, "Chemometrics:  New Tools for Solving Old Problems" presented at the Virginia Commonwealth University, Richmond, VA, January, 20, 1998.

90) P.B. Harrington, "Chemometrics:  New Tools for Solving Old Problems" presented at University of North Carolina, Chapel Hill, NC, February 10, 1997.

91) P.B. Harrington, "Chemometrics:  New Tools for Solving Old Problems" presented at Northern Arizona University, Flagstaff, AZ, November 15, 1996.

92) P.B. Harrington, "Chemometrics:  New Tools for Solving Old Problems" presented at the Arizona State University Department of Chemistry, Tempe, AZ, November 14, 1996.

93) P.B. Harrington, "Chemometrics:  New Tools for Solving Old Problems" presented at the Clemson University Department of Chemistry, Clemson, SC, September 19, 1996.

94) P.B. Harrington, "Making the Connection Between Neural Networks and Analytical Chemistry" presented at De Pauw University, Greencastle, IN, March 14, 1996.

95) P.B. Harrington, "Making the Connection Between Neural Networks and Mass Spectrometry" presented at University of Whales, Swansea, United Kingdom,

August 18, 1995.

96) P.B. Harrington, P. Zheng, P. Tandler, and B. Wabuyele,  "Making the Connection:  Neural Networks and Chemistry" presented at Northern Kentucky University, KY, March 20, 1995.

97) P.B. Harrington, "Making the Connection:  Neural Networks and Chemistry" presented at John Carrol University, Cleveland, OH, October 26, 1994.

98) P.B. Harrington, "Chemometrics:  New Approaches to Solving Old Problems" presented at Xavier University, Cincinnati, OH, September 16, 1994.

99) 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.

100) P.B. Harrington, "New Directions in Analytical Chemistry" guest lecturer in conjunction with the Randolph-Macon Chemistry Department's lecture series, Ashland, November, 1990.

101) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Marshall University, Huntington, WV, March 1990.

102) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Kent State University, Kent, OH, February 1989.

103) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Seton Hall University, East Orange, NJ, March 1990.

104) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Ohio University, Athens, OH, March 1989.

105) P.B. Harrington, "Applications of Pattern Recognition to Pyrolysis Mass Spectrometry," presented at Auburn University, Auburn, AL, March 1989.

106) P.B. Harrington, "Statistical Tests for Analytical Chemists" presented at Utah State University, Logan, UT, March, 1985.

107) P.B. Harrington, "Pyrolysis Gas Chromatography" presented at University of North Carolina, Chapel Hill, NC, March, 1984.

108) P.B. Harrington, "Flavor Modeling Using Headspace and Pyrolysis Gas Chromatography," presented at Randolph-Macon College, Ashland, November, 1981.

109)  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, "A new method of producing highly active oxygen anions and its study on human health", Zhejiang 1000 Scholars Competition, Hangzhou, China, October 17, 2017.

2)  P.B. Harrington, "Application of Support Vector Machines to Chemometrics and the Authentication of Complex Materials", Cannaprint, Inc., Broomfield, CO, January 16, 2016.

3)  P.B. Harrington, "Statistically General Chemometric Models I", IVL Swedish Environmental Research Institute, Stockholm, SE, August 24, 2010.

4)  P.B. Harrington, "Statistically General Chemometric Models II", IVL Swedish Environmental Research Institute, Stockholm, SE, August 24, 2010.

5)  P.B. Harrington, "Statistically General Chemometric Models III", IVL Swedish Environmental Research Institute, Stockholm, SE, August 24, 2010.

6)  P.B. Harrington, "Chemometric Opportunities for the Authentication of Complex Materials", Beltsville Human Nutrition Research Center, USDA/ARS, Beltsville, MD, June 28, 2010.

7)  P.B. Harrington, "Chemometric Opportunities in Forensic Chemical Analysis", Institute of Forensic Science, Ministry of Justice, Shanghai, PRC, April 2, 2009.

8)  P.B. Harrington, "Recruiting Undergraduate Baccalaureate Science Majors", EIC, Group, Shanghai, PRC, April 1, 2009 (teleconference with offices in Beijing, Guangzhou, and Nanjing).

9)  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.

10)  P.B. Harrington, "Bootstrap Methods in MALDI-MS:  How to Get Something from Nothing", National Institutes of Health, Bethesda, MD, November 9, 2006.

11)  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.

12) 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.

13) 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.

14) 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.

15) 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.

16) 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.

17) 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.

18) 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.

19) 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.

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 the National Institutes of Health/National Institute of Child Health and Human Development, Washington DC, May 12, 2004.

21) 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.

22) 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.

23) 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.

24) 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.

25) 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.

26) 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.

27) 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.

28) 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.

29) 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.

30) P.B. Harrington, "Making the Connection Between Neural Networks and Food Analysis" presented at Battelle Columbus, OH, May, 1998.

31) P.B. Harrington, "Making the Connection Between Neural Networks and Food Analysis" presented at Nabisco, East Hanover, NJ, May 14, 1996.

32) 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.

33) 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.

34) P.B. Harrington, P. Zheng, P. Tandler, and B. Wabuyele,  "Making the Connection:  Neural Networks and Chemistry" presented at the National Center for Toxicological Research, Jefferson, AR, April 7, 1995.

35) 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.

36) P.B. Harrington, "Minimal Neural Networks," presented at Leybold Inficon, 2 Technology Place, East Syracuse, NY , March 1992.

37) P.B. Harrington, "Minimal Neural Networks," presented at the National Biscuit Company, East Hanover, NJ  November, 1991.

38) P.B. Harrington, "Minimal Neural Networks," presented at Dow Chemical's Symposium on Neural Network Awareness, Dow Chemical, Freeport, TX, October 1991.

39) 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.

40) P.B. Harrington, "Intelligent Peptide Sequencing," presented at Applied Biosystems, Inc., Foster City, CA, February, 1991.

41) P.B. Harrington, "Fuzzy Rule-Building Expert Systems," presented at Charles Evans and Assoc., Redwood City, CA, February, 1991.

42) P.B. Harrington, "Partial Least Squares Analysis Applied to Property Prediction," presented at Nabisco Brands, Inc. East Hanover, NJ, December, 1989.

43) P.B. Harrington, "Survey of Pattern Recognition Methods," presented at Teledyne CME, Santa Clara, CA, December, 1989.

44) 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 62nd

Annual Meeting, Seattle, WA, February 23, 2010.

**Presentations at International Scientific Conferences**
(*Denotes invited presentation and <u>underlining</u> the presenter)

1) P.B. Harrington*, "Accelerated Restricted Boltzmann Machines Applied to Analytical Chemistry", Topics in Chemometrics, May 17, 2019, Szeged, Hungary, **Keynote.**

2) P.B Harrington*, "Adapted Deep Learning Algorithms for Chemotyping Botanical Medicines", 2$^{nd}$ World Congress on Pharmaceutical and Chemical Sciences (Pharma-2018), July 23, 2018, Bologna, Italy, **Keynote**.

3) P.B. Harrington*, "Cascading and Enhanced Restricted Boltzmann Machines for Feature Expansion of Spectra", Chemometrics in Analytical Chemistry (CAC 2018), Halifax, Canada, June 27, 2018, **Plenary**.

4) <u>P.B. Harrington</u> and Z. Chen, "High-throughput Chemotyping of Cannabis and Hemp Extracts by Ultraviolet Microplate Reader and Multivariate Classifiers", Chemometrics in Analytical Chemistry (CAC 2018), Halifax, Canada, June 25-29, 2018.

5) P.B. Harrington*, "Application of Restricted Boltzmann Machines to Analytical Chemistry", Analytical Chemistry 2018, Vienna, Austria, March 25-28, **Plenary**.

6) P.B. Harrington*, "Enhanced Restricted Boltzmann Machines for Classification of Analytical Measurements", WSC-11 2018, Saint Petersburg, Russia, February 27, 2018, **Plenary**.

7) P.B. Harrington*, "Application of Restricted Boltzmann Machines to the Authentication of Botanical Medicines", Advances in Pharmaceutical Analysis 2017, Wuhan, PRC, November 18, 2017, **Keynote**.

8) P.P. Liu, X. Zhang, B.L. Pan, M.J. Wei, <u>Z. Zhang</u>, 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.

9) 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**.

10) P.B. Harrington*, "Single Set Validation for Classification and Calibration Causes False Conclusions", *5$^{th}$ Annual Congress of Analytix 2017*, Fukuoka, Japan, March 23, 2017, **Keynote**.

11) P.B. Harrington*, "Bootstrapping as a Tool to Automate Chemometric Methods", *Chiométrie XVIII 2017*, Paris, France, January 30, 2017, **Plenary**.

12) P.B. Harrington, "Chemometric Shootout Method Used", *Chiométrie XVIII 2017*, Paris, France, January 30, 2017.

13) 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.

14) 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**.

15) 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.

16) P.B. Harrington*, "Fuzzy Grid Encoding: A New Paradigm for Multivariate Chemometrics", Analytix 2014, Dalian, PRC, April 28, 2014, **Keynote.**

17) P.B. Harrington*, "Smarter Products Based on Chemical Sensing", World Emerging Industries Summit, Wuhan, PRC, November 29, 2013, **Keynote.**

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

19) 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 60th ASMS Conference on Mass Spectrometry and Allied Topics, Vancouver, CA, May 23, 2012, **WP046**.

20) Z. Wang, Y. Zhang, H. Zhang, P.B. Harrington, H. Chen, "Fast and Selective Modification of Thiol Proteins/Peptides by *N*-(Phenylseleno)phthalimide", The 60th ASMS Conference on Mass Spectrometry and Allied Topics, Vancouver, CA, May 22, 2012, **TP128**.

21) P.B. Harrington*, "Fuzzy Optimal Associative Memories for the Authentication of Nutraceuticals by Mass Spectrometry", The 6th Shanghai International

Symposium on Analytical Chemistry, Shanghai, PRC, October 16, 2012.

22) P.B. Harrington*, "Authentication of Foods and Nutraceuticals", 6th International Forum on Food Safety, Shanghai, PRC, September 29, 2011.

23) 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.

24) 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.

25) P.B. Harrington, "Development of Nonlinear Modeling Methods for Chemical Agent Detection from Differential Mobility Images", 17th Annual Conference on Ion Mobility Spectrometry, Ottawa, CA, July 24, 2008.

26) 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.

27) P.B. Harrington*, "Chemometric Opportunities in Proteomic Biomarker Discovery via Mass Spectrometry", Colloquium Spectroscopicum Internationale XXXV, Xiamen, PRC, September 24, 2007.

28) 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**.

29) 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.

30) P.B. Harrington, P. Chen, and A. Yergey, "Theoretical Foundations of Analysis of Variance-Principal Component Analysis", 10th International Conference on Chemometrics in Analytical Chemistry (CAC-2006), Aguas de Lindòia, Brazil, September 12, 2006.

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

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

33) P. Rearden and P.B. Harrington, "Preprocessing of Gas Chromatography Differential Mobility Spectrometry (GC-DMS) Data for Curve Resolution and Classification of Fuels", 3rd Symposium on Computer Applications and Chemometrics in Analytical Chemistry (SCAC-2006), Lake Balaton, Hungary, July 4, 2006.

34) P. Reardon and P.B. Harrington, "Multiway Preprocessing of Gas Chromatography Differential Mobility Spectrometry (GC-DMS) Data for Curve Resolution of Jet Fuels", 14th International Conference on Ion Mobility Spectrometry, Maffliers, France, July 27, 2005.

35) 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", 14th International Conference on Ion Mobility Spectrometry, Maffliers, France, July 25, 2005.

36) 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.

37) 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.

38) 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.

39) 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.

40) P.B. Harrington and Libo Cao, "Modeling Nonlinear Wavelet Compressed Ion Mobility Spectrometry", 12th International Conference on Ion Mobility Spectrometry, Umeå, Sweden, July 28, 2003.

41) P.B. Harrington and Libo Cao, "Tutorial on Modeling and Wavelet Compression for Ion Mobility Spectrometrists", 12th International Conference on Ion Mobility Spectrometry, Umeå, Sweden, July 28, 2003.

42) Z. Zhang*, H. Zhou, S. Liu, and P.B. Harrington, "Classification of Cancer Patients Based on ICP-AES Determinations Using Neural Networks", 9th Beijing Conference and Exhibition on Instrumental Analysis, Beijing, PRC, 2001.

43) 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.

44) P.B. Harrington*, T.L. Buxton, G. Chen, P.J. Rauch, L. Shaw, and A. Urbas, "Strategies for Smarter Chemical Sensors", 7th International Conference on Chemometrics in Analytical Chemistry, Antwerp, Belgium, October 20, 2000.

45) P.B. Harrington, T.L. Buxton, G. Chen, P.J. Rauch, L. Shaw, and A. Urbas, "Chemometric Strategies for Smarter Ion Mobility Spectrometers", 9th International Symposium on Ion Mobility Spectrometry, Halifax, Canada, August 15, 2000.

46) T. Buxton and P.B. Harrington, "Modified Ion Mobility Spectrometer for Enhanced Selectivity", 26th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Vancouver, BC, Canada, October 28, 1999, **705**.

47) P.B. Harrington*, J. Wan, C. Cai, and A. Urbas, "Applications of Neural Networks to Environmental Analysis", 26th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Vancouver, BC, October 27, 1999, **487**.

48) P.B. Harrington* and J. Wan, "Sensitivity Analysis Applied to Artificial Neural Networks:  What has my neural network actually learned?", 8th International Symposium on Ion Mobility Spectrometry, Buxton, United Kingdom, August 9, 1999.

49) P.B. Harrington, "Temperature Constrained-Cascade Correlation Networks", 5th Scandinavian Chemometrics Conference, Lahti, Finland, August 26, 1997.

50) P.B. Harrington, E.S. Reese, P.J. Rauch, C. Wan, and D.M., Davis, "Chemometric Tools for Advantageous Use of Dynamic IMS Data", 6th International Symposium on Ion Mobility Spectrometry, Bastei, Germany, August 14, 1997.

51) P.B. Harrington* and L. Hu, "Copiosity Principle for 21st Century

Chemometricians", Chemometrics in Analytical Chemistry, Tarragona, Spain, June 25, 1996.

52) <u>P. Johnson</u>, L. Hu, E. Saulinskas, and P.B. Harrington, "An Expert System for Amino Acid Sequence Analysis", XIth International Conference on Methods in Protein Structure Analysis, Annecy, FR, September 3, 1996.

53) <u>P.B. Harrington</u>*, P. Zheng, and Dennis Davis, "Automatic Deconvolution-Temperature Constrained Cascade Correlation Neural Networks for Ion Mobility Data Analysis", 4th International Workshop on Ion Mobility Spectrometry, Cambridge, United Kingdom, August 7, 1995.

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

55) <u>P.B. Harrington</u>* 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 <u>underlining</u> the presenter)

1) <u>L. Wang</u>*, M. Vendrell Dones, S. Dogruer, C. Deriu, P.B. Harrington, A. Mebel, B. McCord, "Detection and Quantification of Trace Fentanyl in Mixtures with Portable Raman and Chemometrics", 2020 AAFS Annual Scientific Meeting, Anaheim, CA, February 20, 2020, **Y11**.

2) <u>L. Wang</u>*, M. Vendrell Dones, S. Dogruer, C. Deriu, P.B. Harrington, A. Mebel, B. McCord, "Detection and Quantitation of Fentanyl Mixtures by Surface-Enhanced Raman Spectroscopy and Chemometrics", 2020 AAFS Annual Scientific Meeting, Anaheim, CA, February 18, 2020, NIJ Forensic Science Research and Development (R&D) Symposium.

3) <u>P.B. Harrington</u>*, "Chemometrics for the Masses:  How to Painlessly Improve Your Science", The Eastern Analytical Symposium 2019, Princeton NJ, November 19, 2019, **Harrington Chemometrics Award Symposium**.

4) <u>P.B. Harrington</u>*, "Accelerated Restricted Boltzmann Machines", Federation of Analytical Chemistry and Spectroscopy Societies SciX 2019, Palm Springs, CA, October 17, 2019, **Innovation Award Finalist**.

5) <u>P.B. Harrington</u>*, "Machine Learning for Characterizing and Authenticating Natural Medicines", Federation of Analytical Chemistry and Spectroscopy Societies SciX 2019, Palm Springs, CA, October 16, 2019.

6) <u>P.B. Harrington</u>*, Z. Chen, M. Naderinasrabadi, and J. Staser, "Chemometrics

to Guide the Design of a Lignin Electrocatalytic Reactor", The American Chemical Society Fall Meeting, San Diego, CA, August 29, 2019.

7)  P.B. Harrington*, Z. Chen, M. Naderinasrabadi, and J. Staser, "Chemometrics to Guide the Design of a Lignin Electrocatalytic Reactor", The American Chemical Society Fall Meeting, San Diego, CA, August 29, 2019 (impromptu lecture in Advances in Spectroscopy session).

8)  J. Harnly*, P.B. Harrington*, T. Daniels*, W. Applequist*, and J. Neal-Kababick*, Moderators, P. Brown and H. Johnson, "The Evolution of Analytical Approaches for Botanical Characterization", International Conference of the Science of Botanicals, Oxford, MS, April 18, 2019, **Panel Discussant**.

9)  P.B. Harrington*, "The End of Science, Big Data, and the Rise of Machine Intelligence", Federation of Analytical Chemistry and Spectroscopy Societies SciX 2018, Atlanta, GA, October 26, 2018, **Plenary**.

10)  P.B Harrington*, "Deep Learning Algorithms Applied to Small Spectral Datasets", Federation of Analytical Chemistry and Spectroscopy Societies SciX 2018, Atlanta, GA, October 25, 2018.

11)  Z. Chen*, P.B Harrington, and Z. Zhang, "Diagnosis of Patients with Chronic Kidney Disease by Using Two Fuzzy Classifiers", Federation of Analytical Chemistry and Spectroscopy Societies SciX 2018, Atlanta, GA, October 25, 2018.

12)  Z. Chen and P.B Harrington, "Automatic Soft Independent Modeling of Class Analogy (SIMCA) Using Response Surface Modeling", Federation of Analytical Chemistry and Spectroscopy Societies SciX 2018, Atlanta, GA, October 25, 2018.

13)  Z. Chen and P.B Harrington, "High-throughput Chemotyping of Cannabis and Hemp Extracts by Ultraviolet Microplate Reader and Class Modeling", Federation of Analytical Chemistry and Spectroscopy Societies SciX 2018, Atlanta, GA, October 25, 2018.

14)  P.B Harrington*, "Common Mistakes in Reporting Scientific Results", Federation of Analytical Chemistry and Spectroscopy Societies SciX 2018, Atlanta, GA, October 23, 2018.

15)  P.B. Harrington, "Chemotyping Cannabis by Spectral Fingerprinting", The Science of *Cannabis* 2018, Webinar https://www.analyticalcannabis.com/, September 27, 2018.

16)  D.N. Tabang, A.L. Yergey, P.B. Harrington, F.D. Porter, and S.M. Cologna,

"Mass Spectral Profiling to Identify Cerebrospinal Fluid Markers in Niemann-Pick Disease, Type C1", The 66th ASMS Conference on Mass Spectrometry and Allied Topics, San Diego, CA, June 7, 2018, ThP 046.

17) A. Aloglu and P.B. Harrington, "Differentiation of Bovine, Porcine, and Fish Gelatins", 2018 Ohio University Student Research and Creative Activity Expo, Athens, OH, April 12, 2018.

18) Z. Chen and P.B. Harrington, "High-Throughput Authentication of *Cannabis* Extracts by Ultraviolet Microplate Reader and Multivariate Classifiers", 2018 Ohio University Student Research and Creative Activity Expo, Athens, OH, April 12, 2018.

19) A. Aloglu and P.B. Harrington, "Differentiation of Bovine, Porcine, and Fish Gelatins", 70th Midwestern Universities Analytical Chemistry Conference (MUACC), Athens, OH, October 20, 2017.

20) Z. Chen and P.B. Harrington, "High-Throughput Authentication of *Cannabis* Extracts by Ultraviolet Microplate Reader and Multivariate Classifiers", 70th Midwestern Universities Analytical Chemistry Conference (MUACC), Athens, OH, October 20, 2017.

21) X. Wang and P.B. Harrington, "Optimal Resolution of High-Resolution Mass Spectrometry for the Pattern Recognition of Cannabis Extracts", 70th Midwestern Universities Analytical Chemistry Conference (MUACC), Athens, OH, October 20, 2017.

22) P.B. Harrington, "Application of Restricted Boltzmann Machines to Analytical Chemistry", 70th Midwestern Universities Analytical Chemistry Conference (MUACC), Athens, OH, October 20, 2017.

23) P.B. Harrington, "Multiblock Analysis Using Restricted Boltzmann Machines", Federation of Analytical Chemistry and Spectroscopy Societies SciX 2017, Reno, NV, October 13, 2017 (fill-in).

24) A. Aloglu and P.B. Harrington, "Differentiation of Bovine, Porcine, and Fish Gelatins by Attenuated Total Reflectance Fourier Infrared Spectroscopy (ATR-FTIRS) coupled with Pattern Recognition", Federation of Analytical Chemistry and Spectroscopy Societies SciX 2017, Reno, NV, October 12, 2017.

25) P.B. Harrington*, "Multiple Versus Single Set Validation to Avoid Erroneous Conclusions", Federation of Analytical Chemistry and Spectroscopy Societies SciX 2017, Reno, NV, October 10, 2017.

26) 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.

27) A.K. Aloglu, P.B. Harrington, S. Sahin, and C. Demir, "Chemical Profiling of Floral and Chestnut Honey using High-Performance Liquid Chromatography-Ultraviolet Detection", 2017 Ohio University Student Research and Creative Activity Expo, Athens, OH, April 6, 2017.

28) 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).

29) 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.

30) 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 64th ASMS Conference on Mass Spectrometry and Allied Topics, San Antonio, TX, June 9, 2016, ThOA.

31) 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.

32) 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.

33) 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 16th Annual Oxford International Conference on the Science of Botanicals 5th Interim American Society of Pharmacognosy Meeting (ICSB 2016), Oxford, MS, April 11, 2016.

34) 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.

35) 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.

36) 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**.

37) X. Wang and P.B. Harrington, "Differentiating Rice Varieties by SPME-GC-MS and NMR Chemical Profiling", The 63RD ASMS Conference on Mass Spectrometry and Allied Topics, St. Louis, MO, June 9, 2015, **TP 328**.

38) 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**.

39) 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**.

40) 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 62nd ASMS Conference on Mass Spectrometry and Allied Topics, Baltimore, MD, June 19, 2014, **Th 610**.

41) 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 62nd ASMS Conference on Mass Spectrometry and Allied Topics, Baltimore, MD, June 19, 2014, **Th 561**.

42) X. Wang, and P.B. Harrington, "Differentiating Rice Varieties by Inductively Coupled Plasma/Mass Spectrometry Chemical Profiling", The 62nd ASMS Conference on Mass Spectrometry and Allied Topics, Baltimore, MD, June 18, 2014, **W 343**.

43) Z. Wang, M. Zhang, and P.B. Harrington, "Reconstruction of Mass Spectra Using Fuzzy Optimal Associative Memories (FOAMs)", The 62nd ASMS Conference on Mass Spectrometry and Allied Topics, Baltimore, MD, June 18, 2014, **W 026**.

44) 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.

45) 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.

46) 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 2nd International Conference on Forensic Research and Technology, Las Vegas, NV, October 8, 2013, **974**.

47) 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 61st ASMS Conference on Mass Spectrometry and Allied Topics, Minneapolis, MN, June 13, 2013, **ThP 187**.

48) Z. Wang, P. Chen, L. Yu, and P.B. Harrington.  "Authentication of organic basil plants by using gas chromatography/mass spectrometry chemical profiles", The 61st ASMS Conference on Mass Spectrometry and Allied Topics, Minneapolis, MN, June 13, 2013, **ThP 186**.

49) 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**.

50) 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**.

51) 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**.

52) 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**.

53) 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**.

54)  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**.

55)  P.B. Harrington*, "Chemometric Opportunities for Ion Mobility and Mass Spectrometries", Pittsburgh Mass Spectrometry Discussion Group, Pittsburgh, PA, October 5, 2010.

56)  P.B. Harrington*, "Chemometric Strategies for Authentication of Foods and Herbal Supplements", 124th AOAC Meeting and Exhibition, Orlando, FL, September 29, 2010.

57)  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**.

58)  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**.

59)  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**.

60)  P.B. Harrington*, W. Lu, and Y. Lu, "Novel Algorithm for Registration of Hyperspectral Images and Retention Time Alignment of Multiway Data", 36th Federation of Analytical Chemistry and Spectroscopy Societies, Louisville, KY, October 22, 2009.

61)  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", 123rd Association of Analytical Communities (AOAC) International Annual Meeting & Exposition, Philadelphia, PA, September 14, 2009.

62)  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**.

63) 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**.

64) Weiying Lu and P.B. Harrington, "Radial Basis Function Cascade Correlation Networks", OHIO University Research and Creative Activity Expo, May 14, 2009, **64**.

65) 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**.

66) 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", 35th Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Reno, NV, September 30, 2008.

67) 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**.

68) 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**.

69) 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), New Orleans, LA, March 7, 2008, **2530-7**.

70) 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), New Orleans, LA, March 6, 2008, **2200-8**.

71) 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), New Orleans, LA, March 6, 2008, **1930-3**.

72) 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), New Orleans, LA, March 5, 2008, **1490-8**.

73) 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), New Orleans, LA, March 5, 2008, **1440-2**.

74) 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), New Orleans, LA, March 5, 2008,**1170-3**.

75) 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), New Orleans, LA, March 4, 2008, **430-5**.

76) 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**.

77) 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**.

78) 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**.

79) 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.

80) 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.

81) 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**.

82) 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**.

83) 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**.

84) 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[td] Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Lake Buena Vista, FL, September 27, 2006.

85) P.B. Harrington*, "Two-way Multivariate Correlation as an Information Theoretic Tool for Measuring Analytical Orthogonality" presented at The 33[td] Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Lake Buena Vista, FL, September 25, 2006.

86) 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.

87) 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.

88) 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.

89) 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.

90)  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.

91)  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.

92)  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**.

93)  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**.

94)  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**.

95)  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**.

96)  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 **580-2580-3**.

97)  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**.

98)  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.

99)  P. Rearden and <u>P.B. Harrington</u>, "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.

100)  <u>P. Rearden</u> 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.

101)  <u>P. Chen</u> 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**.

102)  <u>P. Rearden</u> 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**.

103)  <u>P.B. Harrington*</u>, 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.

104)  <u>A.L. Yergey*</u>, 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.

105)  <u>P. Chen*</u> 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.

106)  <u>P.B. Harrington</u> and P. Chen, "Equilibrium Modeling of Ion Mobility Spectra", presented at The 13th International Conference on Ion Mobility Spectrometry, Gatlinburg, TN, July 29, 2004.

107)  <u>M.L. Ochoa</u> 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.

108) 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.

109) 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.

110) 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.

111) 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.

112) 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**.

113) 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**.

114) 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**.

115) 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**.

116) 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**.

117) P.B. Harrington and L. Cao, "Chemometric Modeling of Mass Spectra", presented at the 2nd Ohio Analytical Chemistry Consortium, Columbus, OH, October 31, 2003.

118) A.K. Gianatto, J.W. Rawlinson, K.C. Cossel, P.B. Harrington, A.D. Appellhans, 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.

119) 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**.

120) 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**.

121) 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**.

122) 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**.

123) P.B. Harrington*, "Chemometrics Opportunities in Ion Mobility and Mass Spectrometries" presented at The 1st Ohio Analytical Chemistry Consortium, Columbus, OH, November 8, 2002.

124) 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.

125) 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.

126)   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**.

127)   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.

128)   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.

129)   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**.

130)   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**.

131)   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,  T**PK291**.

132)   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**.

133)   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**.

134) <u>G. Chen</u> 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**.

135) <u>G. Chen</u> 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**.

136) <u>P.B. Harrington*</u>, 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.

137) <u>P.B. Harrington*</u>, 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**.

138) <u>A. Mehay</u> 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**.

139) <u>J.M. Perr</u> 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**.

140) <u>M.L. Patchett</u> and P.B. Harrington, "Detection of Gamma Hydroxybutryate Using Ion Mobility Spectrometry," The 52nd Pittsburgh Conference and Exposition on Analytical Chemistry & Applied Spectroscopy, New Orleans, LA, March 8, 2001, **1067**.

141) <u>T.L. Buxton</u> 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**.

142) <u>G. Chen</u> 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**.

143) K.J. Voorhees and <u>P.B. Harrington*</u>, "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.

144) 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**.

145) 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**.

146) 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**.

147) 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**.

148) 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**.

149) 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**.

150) 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**.

151) 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**.

152) 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**.

153) 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**.

154) <u>T.L. Buxton</u>, and P.B. Harrington, "Modified Ion Mobility Spectrometer for Enhanced Selectivity" presented at The 1999 Pittsburgh Conference, Orlando, FL, March 9, 1999, **601**.

155) <u>L.A. Shaw</u> 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**.

156) <u>C. Cai</u> 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**.

157) <u>C. Wan</u> 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**.

158) <u>C. Cai</u> 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**.

159) <u>P.B. Harrington</u>*, "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**.

160) <u>C. Wan</u> 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.

161) <u>D.M. Davis</u>*, 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.

162) <u>P.B. Harrington</u>*, L. Hu, and C. Cai, "Recovery of Variable Loadings and Eigenvalues Directly form Fourier Compressed Data" presented at ISIMS '98, Hilton Head, SC, August 10, 1998.

163) <u>C. Cai</u> and P.B. Harrington*, "Linear Discriminant Classification of Fourier and Wavelet Compressed IMS Data" presented at ISIMS '98, Hilton Head, SC, August 10, 1998.

164) <u>J. Stotz</u> and P.B. Harrington, "Accellerant Detection for Arson Investigations

Using Ion Mobility Spectrometry" presented at Pittcon '98, New Orleans, LA, March 4, 1998, 884.

165)   E. Horak and P.B. Harrington, "Calibration and Characterization of a Vapor Generator" presented at Pittcon '98, New Orleans, LA, March 4, 1998, 847.

166)   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.

167)   C. Cai and P.B. Harrington, "Enhanced Temperature Constrained Cascade Correlation Networks" presented at Pittcon '98, New Orleans, LA, March 2, 1998, 383.

168)   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.

169)   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.

170)   P.B. Harrington*, "Evaluation of Data and Model Quality" presented at the Optical Society of America Annual Meeting, Long Beach, CA, October 14, 1997.

171)   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, Jekyl Island, GA, June, 1997.

172)   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.

173)   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.

174)   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.

175) 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.

176) 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.

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178) 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.

179) P.B. Harrington*, "Chemometric Approaches to Micromachined Analysis" presented at the First OMACC Symposium, Miami University, Oxford, OH, September 5, 1996.

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181) 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.

182) 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.

183) 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.

184) 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.

185) 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

186) <u>L. Hu</u>, 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.

187) <u>P. Zheng</u> 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.

188) 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.

189) P.B. Harrington*, "Temperature Constrained-Cascade Correlation Neural Networks" presented at the Ohio Aerospace Institute Neural Networks 1995 Symposium, Athens, OH, August 21, 1995.

190) <u>P. Zheng*</u> 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.

191) <u>L. Hu</u>, 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.

192) <u>P.B. Harrington</u> and B. Wabuyele, "Fuzzy Optimal Associative Memory for Background Prediction of Spectra" presented at The 1995 Pittsburgh Conference, New Orleans, LA, March 1995, 711.

193) <u>P.J. Tandler</u>, 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.

194) <u>P.J. Rauch</u> 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.

195) <u>P.B. Harrington</u> 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.

196) P.B. Harrington*, "Making the Connection:  Neural Networks and Chemistry" presented at The Cleveland Section of the American Chemical Society/Society

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197) 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.

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201) 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.

202) 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.

203) D. Wuersig and P.B. Harrington, "Quantitative Spectra-Retention Relationships" presented at The 1994 Pittsburgh Conference, Chicago, IL, March 1994, 792.

204) 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.

205) 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.

206) 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.

207) P.B. Harrington, "Optimal Fuzzy Decision Making" presented at The 1994

Pittsburgh Conference, Chicago, IL, March 1994, 640.

208)  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.

209)  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.

210)  P.B. Harrington, "Optimal Fuzzy Decisions for Problems in Analytical Chemistry." presented at the Midwestern University Analytical Chemistry Conference, IndianaUniversity, Bloomington, IN, October 15, 1993.

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212)  P.B. Harrington*, "Neural Networks Applied to Analytical Chemistry" presented at the OhioUniversity$\Sigma$X May Meeting, Athens, OH May 1993.

213)  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.

214)  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.

215)  H. Whittenburg, D. King, B.W. Wabuyele 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.

216)  B.W. Wabuyele 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.

217)  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.

218)  P.B. Harrington, "Constrained Learning Algorithms for Backpropagation Neural

Networks:  Local Temperature Maximization" presented at the 1993 Pittsburgh Conference, Atlanta, GA, March 1993, 368.

219)  P. Zheng and P.B. Harrington, "Cluster Analysis of Secondary Ion Mass Spectra" presented at the 1993 Pittsburgh Conference, Atlanta, GA, March 1993, 039.

220)  P.B. Harrington*, "Minimal Neural Networks:  Temperature Jump Training" presented at Federation of Analytical Chemistry and Spectroscopy Societies XIX, Philadelphia, PA, September, 1992.

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222)  B. Wabuyele 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.

223)  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.

224)  P.B. Harrington, "Minimal Neural Networks:  Concerted Optimization of Multiple Linear Discriminants," presented at the 1992 Pittsburgh Conference, New Orleans, LA, March, 1992, 174.

225)  P.B. Harrington, "Minimal Neural Networks," presented at the Eastern Analytical Symposium, Somerset, NJ November, 1991.

226)  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.

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229)  P.B. Harrington, "Fuzzy Rule-Building Expert System:  Minimal Neural Network" presented at the 1991 Pittsburgh Conference, Chicago, IL, March, 1991, 562.

230) P.B. Harrington*, "Digital Distributed Parallel Processing," presented at Federation of Analytical Chemistry and Spectroscopy Societies XVII, Cleveland, OH, October, 1990, 843.

231) P.B. Harrington*, "Fuzzy Rule Building Expert Systems," presented at the Third Hidden Peak Symposium on Computer-Enhanced Analytical Spectroscopy, Snowbird, UT, June, 1990.

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