Curriculum Vitae

Steven D. Brown
Willis F. Harrington Professor
Department of Chemistry and Biochemistry
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EXPERTISE

Chemical data analysis, including signal processing and detection, background removal, and transfer of multivariate calibrations. Data mining and knowledge discovery of chemical relationships involving multivariate data, including development of novel classifiers and hierarchical classification methods. Fusion of chemical sensor data for classification and calibration.

ACADEMIC TRAINING

Postgraduate:
Attended NATO Advanced Study Institute on Chemometrics, Cosenza, Italy, 1983
Invited Participant at Chemistry Research Applied to World Needs (CHEMRAWN) IV:
Chemistry applied to Oceanography, Keystone, Colorado, 1987.

Graduate:
University of Washington
Seattle, Washington
1975-1978, Ph.D. (G.P.A. 4.00/4.00)
Major: Analytical Chemistry
Thesis Topic: Computer-Controlled Electrochemistry and Pattern Recognition
Thesis Director: B.R. Kowalski

Portland State University
Portland, Oregon
1973-1975, M.A. (G.P.A. 4.00/4.00)
Major: Physical-Inorganic Chemistry
Thesis Topic: Synthesis and Spectral Characterization of Transition Metal Fluorides
Thesis Director: G.L. Gard

University of British Columbia
Vancouver, British Columbia, Canada (G.P.A. 88 marks -First Class Honours; 88 = 4.00 on American 4 pt grading scale)
1972-1973, left to support mother on death of father
Major: Physical - Inorganic Chemistry, INSERC Fellow

Undergraduate:

Portland State University
1968-1972, B.S., Summa cum laude (G.P.A. 3.93/4.00)
Major: Chemistry, Minor: Physics

RESEARCH AND TEACHING EXPERIENCE

Research and Teaching:
2012	Sabbatical Visitor, Irstea, Montpellier, France
2005-2011	Chair, University of Delaware Institutional Animal Committee on Use and Care (IACUC)
2002-present	Willis F. Harrington Professor, University of Delaware
1997-2002	Chairman, Dept. of Chemistry and Biochemistry, University of Delaware
1997-present	Professor, University of Delaware
1994	Sabbatical Visitor, Technical University of Vienna, Vienna, Austria
1986 -1997	Associate Professor, University of Delaware.
1984 -1985	Associate Professor, Washington State University.
1981-1984	Assistant Professor, Washington State University.
1978-1981	Assistant Professor, University of California at Berkeley.
1978-1981	Principal Investigator (joint appointment), Lawrence Berkeley Laboratory.
1974-1975	Instructor in Chemistry, Mt. Hood Community College.

Short Courses:
2012	Lecturer, Chemometrics Seminar Series, Irstea, Montpellier, France
2006	Lecturer, Short Course on Chemometrics, Kraft Foods, Glenview IL
2005	Lecturer, ACS-PRF Summer School in Chemometrics, Atlanta, GA
1999	Lecturer, Short Course on Chemometrics, GE Plastics, Evansville, IN
1999	Lecturer, Short Course in Chemometrics, Allied Signal, Morrisville, NJ
1997-99	Lecturer, Short Course in Chemometrics, Foss NIRSystems, Silver Spring, MD
1997	Lecturer, Short Course in Chemometrics, Monsanto, St. Louis, MO
1997-98	Lecturer, Short Course in Chemometrics, DuPont, Wilmington, DE
1996 –98	Lecturer, EAS Short Course "Chemometric Calibration through Examples" (With B. Lavine)
1995, 1997	Lecturer, Short Course in Chemometrics, Exxon Research, Florham Park, NJ.
1994	Lecturer, Short Course in Chemometrics, Technical University of Vienna, Vienna, Austria
1992 – 2007	Lecturer, ACS Short Course "Winning at Chemometrics" (with B. Lavine)
1992	Lecturer, Short Course in Chemometrics, Baxter-Paramax, Irvine, CA.
1988-1992	Lecturer, Short Course on Chemometrics, FACSS Conference (with B. Lavine)
1990	Lecturer, Short Course on Chemometrics, Hercules Chemical Corporation, Wilmington, DE.
1988	Lecturer, Short Course on Chemometrics, Scientific Computing and Automation Conference, Philadelphia, PA.

HONORS AND AWARDS

2015 Kowalski Award (John Wiley Publishers), Best Applied Chemometrics Paper (With B. Lavine, A. Fasasi, N. Mirjankar, M. Sandercock)

2015 UMBC Research Symposium, 1st Place Poster, Chemistry Division (with C. Giglio)
2015 Appointed to Editorial Board, Nature Scientific Reports
2013 Success Story Presentation, NURI Conference, Washington, DC
2011 National Geospatial Agency-National Academic Research Program Conference Award, Best Presentation.
2009 UMBC Research Symposium, 1st Place Poster, Biology Division (with T. Bazzoli)
2008 UMBC Research Symposium, 1st Place Poster, Biology Division (with T. Bazzoli)
2002 Appointed Willis F. Harrington Professor, University of Delaware
2002 Scientific Advisory Board, InfraredX, Cambridge, MA.
2001 EAS Prize for Best Poster Paper in Spectroscopic Methods (with H.-W. Tan)
1997 Appointed Chairman, Department of Chemistry and Biochemistry (5 yr. term)
1997 Granted Promotion to Professor, University of Delaware
1996 EAS Award in Chemometrics (first recipient)
1994 Appointed Editor-in-Chief, Journal of Chemometrics
1989 Appointed Chemometrics Series Editor, CRC Press
1989 Appointed Editor (North America), Journal of Chemometrics
1987 Invited participant, CHEMRAWN IV, Keystone, Colorado
1987 Appointed to Editorial Board, Analytica Chimica Acta
1985 Appointed Associate Editor (North America), Journal of Chemometrics
1984 Granted Tenure and Promotion to Associate Professor, Washington State University
1979 Appointed to Editorial Board, Analytical Letters (Chemometrics Section)
1979 U.C. Regents Junior Faculty Fellowship
1978 U.W. Graduate School Award for Graduate Research
1977-1978 Stout Fellowship (University of Washington)
1977-1978 A.C.S. Analytical Chemistry Division Fellowship (Perkin Elmer)
1975 Full Member, Sigma Xi

PROFESSIONAL AFFILIATIONS

Offices held:

Editorial Board, Journal of Chemometrics, 2007-present
Editorial Board, Nature Scientific Reports, 2015-2016
Editor-in-Chief, Journal of Chemometrics, 1994-2007
Member, Scientific Board, InfraredX, Cambridge, MA, 2002-2006
Associate Editor for Chemometrics, Analytical Letters, 1992 - 1994
Editor, CRC Press Series on Chemometrics, 1989-1995
Invited Contributing Member, Chemtracts, 1989-1990 (journal was discontinued in 1990)
North American Editor, Journal of Chemometrics, 1986-1994
Member, Editorial Board, Analytica Chimica Acta, 1987-1993
Member, Editorial Board, Analytical Letters, Chemometrics Section, 1978-1993
IUPAC Working Group on Chemometrics, 1987-present (Representative from U.S.A.)
International Chemometrics Society
        Officer in charge of Course Accreditation, 1988-present
        President of the North American Chapter, 1990-92
American Statistical Association, Chemstatistics Committee, 1987-95
 American Chemical Society, Washington-Idaho Border Section
        Secretary-Treasurer, 1982-1983

Vice-Chair, 1983-1984
Chairman, 1984-1985

Memberships:
American Chemical Society, Analytical Chemistry Division and Computers in Chemistry Division
Chemometrics Society
Sigma Xi
American Statistical Association

Reviewer for:

Journals:
Nature, Science, Analytical Chemistry, Analytica Chimica Acta, Applied Spectroscopy, Analytical Letters, Chemometrics and Intelligent Lab Systems, Clinical Chemistry, J. Chemometrics, Industrial and Engineering Chemistry, Chemical Engineering, J. Chromatography, J. Physical Chemistry, Talanta, Journal of Chemical Information and Computer Science, Microchemical Journal, Biometrika, Technometrics, Analyst, Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, J Mass Spectrometry, Fuel, IEEE journals, PLOS One, Nature, Nature Scientific Reports, Computer Methods and Programs in Biomedicine, many others.

Publishers:
US National Academy of Sciences, Elsevier Scientific, John Wiley and Sons, Verlag Chemie, Prentice Hall, CRC Publishing, Academic Press, Harcourt, Mosby-World Book, Cambridge Scientific, Springer, Oxford Scientific, ACS Publications.

Granting Agencies:
Department of Energy, National Science Foundation (chemistry, engineering and statistics sections), Small Business Initiative Research, NIH, Cottrell Research Foundation, Petroleum Research Fund, National Research Council of Canada, Fund for Former Soviet Bloc Scientists, Netherlands Organisation for Scientific Research (NWO), Volkswagen Stiftung, Velux Fondene

Universities:
Referee on Promotion and Tenure, University of Alaska (Prof. John Kennish), 1982.
Referee on Promotion, University of Alaska (Prof. John Kennish), 1985.
External Departmental Reviewer, Chemistry, University of Idaho, 1984-85.
Referee on Promotion and Tenure, East Carolina University (Prof. Paul Gemperline), 1988.
Referee on Promotion and Tenure, Virginia Commonwealth University (Prof. Sarah C. Rutan), 1990.
External Departmental Reviewer, Statistics, University of Kentucky, 1990
Referee on Tenure, Clemson University (Prof. Ron Williams), 1991
Referee on Appointment to Boyd Professorship, Louisiana State University System (Prof. George G. Guilbault), 1991
Referee on Promotion and Tenure, Clarkson University (Prof. Barry Lavine), 1991
Referee on Promotion and Tenure, University of Tennessee, Dept. of Electrical and Computer Engineering (Prof. Paul B. Crilly), 1991
Referee on Promotion, St. John's University (Prof. Neil Jespersen), 1991

Referee on Promotion and Tenure, University of Louisville, (Prof. M. Cecelia Yappert), 1991.
Referee on Promotion and Tenure, University of Kentucky, Dept. of Statistics, (Prof. William S. Rayens), 1991.
Referee on Appointment to Congressional Fellow, University of Tennessee, Dept. of Electrical and Computer Engineering (Prof. Paul B. Crilly), 1993.
Referee on Promotion and Tenure, Dalhousie University (Prof. Peter Wentzell), 1993.
External Departmental Reviewer, Southern Louisiana University, 1993.
Referee on Promotion, Idaho State University, Department of Mathematics (Prof. Patrick Lang), 1994.
Referee on Promotion, Clemson University (Prof. Ron Williams), 1996
Referee on Promotion and Tenure, University of California, Riverside (Prof. Sharon Neal), 1997
Referee on Appointment to Distinguished Professor, East Carolina University (Prof. Paul Gemperline), 1997.
Referee on Appointment to Senior Lecturer, University of Bristol (Dr. Richard Brereton), 1997.
Referee on Appointment to Distinguished Professor, East Carolina University (Prof. Paul Gemperline), 2001.
Referee on Promotion and Tenure, Arizona State University (Prof. Karl Booksh), 2001.
Referee on Promotion, Dalhousie University (Prof. Peter Wentzell), 2001.
Referee on Promotion, Ohio University (Prof. Peter Harrington), 2001.
Referee on Appointment to Distinguished Research Professor, University of Antwerp (Prof. Piet VanEspen), 2005.
Referee on Promotion and Tenure, Merrimack University (Prof. Steve Theberge), 2005.
Referee on Promotion, Arizona State University (Prof. Karl Booksh), 2005.
Referee on Promotion, University of Kentucky, Dept. of Statistics (Prof. William S. Rayens), 2005.
Referee on Promotion, SLU, Uppsala, Sweden (Prof. Paul Geladi), 2007
Referee on Promotion to University Professor, Dalhousie University, Halifax, NS, Canada (Prof. Peter Wentzel)
Referee on Promotion and Tenure, University of Tennessee (Prof. Frank Vogt), 2010
Referee on Rasmussen Chair, Royal University, Copenhagen, Denmark (Prof. Rasmus Bro), 2012
Referee on W2 Lichtenberg Professor, Universität Jena, Jena, Germany, (Prof. Jan Baumbach), 2014.
Referee on appointment to Professor, University of Balouchistan, Pakistan (Prof. M. Khattak)
Referee on appointment to Professor, Jordan University of Science and Technology, Jordan (Prof. S.A. Barakat)
Referee on appointment to Professor, University of Tennessee (Prof. F. Vogt), 2017

Societies:
Member, ACS Electrochemistry Award Committee, 1989-1992. Committee Chair, 1992.
Member, ASA Statistics-Chemistry Joint Research Award Committee, 1990-99.
Member, EAS Chemometrics Award Jury, 1997-2000, 2010, 2012, 2014, 2015. Jury Chair, 2000.
Member, Kowalski Chemometrics Award Jury, 1999-2004, 2007, 2011-2017. Chair 1999-2002

Consultant to:

ITT Industries 2004-2005
Geomet, 2003-2004
InfraredX, 2002-2006
Gore 1995-2002

Allied Signal-Honeywell 1998-2000
Bayer HealthCare 1998-2011
SmithKline French Laboratories, 1986-1988.
Mobil Oil Corp., 1988
Princeton Applied Research, 1988
DuPont de Nemours, Inc., 1988, 1990-1992, 2002-2011
Hercules, Inc., 1989-1991
Exxon, 1990 - 1991
ICI Pharmaceuticals (Zeneca) 1990-1991, 1993-4, 2005
Microbial Identification Incorporated (MIDI), 1991, 1995-97
MESH, Inc., 1991-1993
Baxter HealthCare, 1992-1993
Science and Technology Corp., 1993-1994
W.R. Grace, 1993
Elf Atochem, 1993-98
Battelle RTP, 1993-1995
NIRSystems, 1993-1995, 1997-99
CECOM 1993-2004
BioControl Technology, 1996-97
Educational Testing Service, 1996, 2002-present
Astra Zeneca, 2005-2007.
CENTRA, 2005
Isense, 2014-2015 (Company closed 2015)

GRANTS AND CONTRACTS

2015-2019 National Science Foundation, Chemical Measurement and Imaging Section, Chemistry Division, "Collaborative Research: Variable Selection for Remedying the Effects of Uncontrolled Variation in Data Driven Predictions," CHE-1506853, $780K total, $520K is UD share. (With K. Booksh (UD), B. Lavine (OSU)).

2015-2017   National Geospatial Intelligence Agency; National University Research Initiative "Propagating/Ascertaining Uncertainty in Hierarchical, Tree-Structured Models" $150K for GY 2016-2017, $300K for 2015-2017.

2009-2014 National University Research Initiative NGA "Estimating Class Uncertainties in Multivariate Geospatial Data" $150K for GY 2012-2013, $600K for 2009-2014.

2010-2011 US Dept. of Justice/Oklahoma State University, "Improving Investigative Lead Information and Evidential Significance Assessment for Automotive Paint and the PDQ Database," $25K.

2009-2012 Biogen IDC, "Bayesian and Fusion Methods for Assessment of Spectral Relationships" , $80K total; $30K for GY 2011-12.

1999-2009 Center for Process Analytical Chemistry, "Novel Classification Tools Combining Data Mining And Statistical Inferencing Techniques", Total Award is $210K.

1996-2009 Center for Process Analytical Chemistry, "Novel Methods for Transfer of Multivariate Calibration," Total Award is $340K

2005-07 Bayer HealthCare, "Determination of Clinically Relevant Analytes in Vitro and in Vivo," $120.8 K.

2003-04 Defense Advanced Research Projects Agency   "How do MHC Genes Determine Chemosensory Individuality?" With Konrad Lorentz Institute, Vienna, University of Newcastle, UK, and Indiana University; UD Share $72K

2003-04 Astra-Zeneca, Inc. "Updating and Transfer of Multivariate Calibrations and Classification", $22.0K

2002-04 W.L. Gore, Inc. "Novel Classification Tools," $58K.

2002-03 US Army ERDEC "Novel methods for Data Analysis," $67K.

1998-2005 Bayer Diagnostics "Calibration Studies," Unrestricted Research Grants, $150K

2001-03 Acquisition of X-Ray Diffractometer, NSF-CRIF, $170K, with A. Rheingold, others.

1999-00 DuPont de Nemours, Inc., "Applications of FIR Transfer of Multivariate Calibration," Unrestricted Research Grant $10K.

1999   Rohm and Haas, Inc. "Transfer of Calibration," Unrestricted Research Grant, $10K.

1998   DuPont de Nemours, Inc., "New Methods for Transfer of Multivariate Calibration," Unrestricted Research Grant $10K.

1998   Dow Chemical Co., "Transfer of Calibration," Unrestricted Research Grant, $10K

1996-9 State of Delaware "Advanced Technology Center", $560K per year in FY 1996-9. Joint project with Microbial ID, Inc., Scientific Computing Solutions, Inc., Berger Instruments and Hewlett - Packard, Inc. UD share for FY 1999-00 is $55.8 K. Total UD funding was $167.4K.

1996   Dow Chemical Co., "Transfer of Calibration", Unrestricted Research Grant, $7K.

1995   DuPont de Nemours, Inc., "Novel Methods for Transfer of Multivariate Calibration," Unrestricted Research Grant $10K.

1994-5 Department of the Army, "Analysis of Pyrolysis Mass Spectral Responses," $84.1 K.

1993-4 Department of the Army, "Analysis of Pyrolysis Mass Spectral Responses," $74.9 K.

1992-5 National Science Foundation, "Student-Based Consulting Program in Chemical Analysis", $75 K, matched with $75K from University of Delaware (with M. V. Johnston)

1992-3 Department of the Army, "Signal and Data Processing with Neural Networks,"$50.0 K.

1991-2 Department of the Army, "Signal Processing of Time-Resolved Pyrolysis MS Data", $49.0 K.

1991   Department of the Army, "Multivariate Analysis of Pyrolysis MS Data", $30.0K.

1991   ARCO Chemical Co. "Quantitative and Qualitative Analysis by Ultrasound", $10K.

1984-7 Department of Energy, "Studies of the Analyte-Carrier Interface in Flow Injection Analysis", $78.8K.

1989   Department of the Army, "Real-Time Analysis of Interferometric Data", $6K.

1987-90 Department of Energy, "Studies of the Analyte-Carrier Interface in Flow Injection Analysis", $234.5K.

1987   University of Delaware Research Foundation", Chemical Matrix and Mixed Interface Effects in Multicomponent Quantitative Analysis",$14K.

1985   National Science Foundation, "Acquisition of a Fourier Transform Infrared Spectrometer", $85K. (with K.W. Hipps).

1986-91 Department of Energy, "Studies of the Analyte-Carrier Interface in Flow Injection Analysis", $198K.

1983-4 Washington State University Research Grant, "Multicomponent Flow Analysis", $8.5K.

1983-4 National Science Foundation, "Acquisition of a GC-Mass Spectrometer", $120K (with H.H. Hill, others).
1978-81 Department of Energy, "Thermodynamic Properties of Actinide Species in Dilute Solution", continuing contract, FY 1981 funding, $301K. (with N. Edelstein). Total funding $731K.

1978-81. Department of Energy, "Analysis of Trace Actinides and Metals in Environmental Samples", $150K.

1978-81. Petroleum Research Fund, "Studies of Hydrodynamic Electrochemistry",$10K.

1979   University of California Research Grant, "Speciation by Raman Spectroscopy", $7K

REFEREED PUBLICATIONS

1.   S.D. Brown and G.L. Gard, "The Chemistry of Chromyl Fluoride, II, " Inorg. Chem., 12, 483-484 (1973).
2.   S.D. Brown and G.L. Gard, "New Preparation of Peroxydisulfuryl Difluoride," Inorg. Nucl. Lett., 11, 19-21 (1975).

3.   S.D. Brown and G.L. Gard, "Reaction of Chromyl Trifluoroacetate with Strong Acids," Inorg. Chem., 14, 2273-2274 (1975).

4.   S.D. Brown and G.L.Gard, "The Reaction of Chromium Trioxide and Metal Oxide Salts with Pyrophosphoryl Tetrafluoride," J. Inorg. Nucl. Chem., 37, 2557-2558 (1975).

5.   S.D. Brown, P.J. Green and G.L. Gard, "The Chemistry of Chromyl Fluoride. III. Reactions with Inorganic Systems," J. Fluorine Chem., 5, 203-220 (1976).

6.   S.D. Brown and G.L. Gard, "The Chemistry of Chromium Pentafluoride. II. Reactions with Inorganic Systems," J. Fluorine Chem., 7, 19-32 (1976).

7.   S.D. Brown, T.M. Loehr and G.L. Gard, "The Vibrational Spectrum of Chromium Pentafluoride," J. Chem. Phys., 64, 260-262 (1976).

8.   S.D. Brown, T.M. Loehr and G.L. Gard, "The Chemistry of Chromyl Fluoride. IV. Raman Spectra of Chromyl Fluoride in the Solid and Liquid Phases," J. Chem. Phys., 64, 1219-1222 (1976).

9.   S.D. Brown, "Zeeman Effect-Based Background Correction in Atomic Absorption Spectroscopy," Anal. Chem., 49, 1269A-1281A (1977).

10.   S.D. Brown and G.L. Gard, "Oxidation of Transition Metal Carbonyls by Peroxydisulfuryl Difluoride," Inorg. Chem., 17, 1363-1364 (1978).

11.   S.D. Brown, J.D.S. Danielson, C.J. Appellof and B.R. Kowalski, "A General Purpose Interface for the PDP-11 Minicomputer," Chem. Biomed. And Environ. Instrum., 9, 29-47 (1979).

12.   S.D. Brown and B.R. Kowalski, "Minicomputer-Controlled, Background-Subtracted Anodic Stripping Voltammetry: Evaluation of Parameters and Performance," Anal. Chim. Acta, 107, 13-27 (1979).

13.   S.D. Brown and B.R. Kowalski, "Pseudopolarographic Determination of Metal Complex Stability Constants by Computer-Controlled Voltammetry," Anal. Chem., 51, 2133-2139 (1979).

14.   S.D. Brown, B.R. Kowalski and R.K.Skogerboe, "Assessment of the Impact of Coal Mining on Water Quality by Pattern Recognition," Chemosphere, 9, 265-276 (1980).

15.   J.J. Toman, R.M. Corn and S.D. Brown, "Convolution Voltammetry of Metal Complexes," Anal. Chim. Acta, 123, 87-199 (1981).

16.   J. J. Toman and S.D. Brown, "Peak Resolution by Semiderivative Voltammetry," Anal. Chem., 53, 1497-1504 (1981).

17.   T.F. Brown and S.D. Brown, "Resolution of Overlapped Electrochemical Peaks with the Use of the Kalman Filter," Anal. Chem., 53, 1410-1417 (1981).

18.   T.F. Brown, D.M. Caster and S.D. Brown, "Speciation of Labile and Quasi-Labile Metal Complex Systems Using the Kalman Filter," NBS Special Publication 681, 163-172 (1981).

19.   S.C. Rutan and S.D. Brown, "Pulsed Photoacoustic Spectroscopy and Spectral Deconvolution with the Kalman Filter for Determination of Metal Complexation Parameters," Anal. Chem., 55, 1707-1710 (1983).

20.   D. Caster and J.J. Toman and S.D. Brown, "Curve Fitting of Semiderivative Linear Scan Voltammetric Responses: Effect of Reaction Reversibility," Anal. Chem., 55, 2143-2147 (1983).

21.   T.F. Brown, D.M. Caster and S.D. Brown, Parameter Estimation Using the Kalman Filter: Heterogeneous Charge Transfer Kinetics," Anal. Chem., 56, 1214-1221 (1984).

22.   S.C. Rutan and S.D. Brown, "In-Situ Pulsed Photoacoustic Spectroscopy and Selective Determination of Sorbed and Solution Praseodymium Species," Anal. Chim. Acta, 158, 113-117 (1984).

23.   S.C. Rutan and S.D. Brown, "Model Error Compensation in Multi-Component Analysis Using Adaptive Kalman Filtering," Anal. Chim. Acta, 160, 99-119 (1984).

24.   C.A. Scolari and S.D. Brown, "Resolution of Strongly Overlapped Responses in Square-wave Voltammetry Using the Kalman Filter" Anal. Chim. Acta, 166, 253-260 (1984).

25.   S.C. Rutan and S.D. Brown, "Simplex Optimized Adaptive Kalman Filter," Anal. Chim. Acta, 167, 39-50 (1985).

26.   S.C. Rutan and S.D. Brown, "Estimation of First-order Kinetic Parameters Using the Extended Kalman Filter," Anal. Chim. Acta, 167, 23-37 (1985).

27.   S.C. Rutan and S.D. Brown, "Two-Dimensional and Three-Dimensional Analysis of Kinetic Systems Using the Extended Kalman Filter," Anal. Chim. Acta, 175, 219-229 (1985).

28.   S.D. Brown and S.C. Rutan, "Adaptive Kalman Filtering," NBS J. Research, 90, 403-407 (1985).

29.   C.A. Scolari and S.D. Brown, "Multicomponent Analysis in Flow Injection Analysis with Square Wave Detection Using the Kalman Filter," Anal. Chim. Acta, 178, 239-246 (1985).

30.   S.D. Brown, "The Kalman Filter in Analytical Chemistry: Principles and Practical Applications," Anal. Chim. Acta, 181, 1-26 (1986).

31.   S.D. Brown, "Chemical Measurements and Data Reduction from a Systems Analysis Perspective," TrAC, 6(10) 260-266 (1987).

32.   S.L. Monfre and S.D. Brown, "Kalman Filtering of First-Order Chemical Kinetics using Fourier Transform Infrared Spectroscopic Data," Anal. Chim. Acta, 200, 397-410 (1987).

33.   T.Q. Barker, H.R. Wilk, S.L. Monfre and S.D. Brown, "Multicomponent Analysis in Static and Flow Systems using Digital Filters," NBS J. Research, 93, 253-5 (1988).

34.   T.Q. Barker and S.D. Brown, "Estimation of Second-Order Kinetic Parameters Using the Extended Kalman Filter," J. Chemometrics, 2, 137-154 (1988).

35.   S.D. Brown, T.Q. Barker, R.A. Larivee, S.L. Monfre, and H. Wilk, "Chemometrics: Fundamental Review, Anal. Chem., 60, 252-274R (1988).

36.   T.Q. Barker and S.D. Brown, "Analysis of a Co-eluting Chromatographic Pair in Liquid Chromatography", Journal of Chromatography, 469, 77-90 (1989).

37.   H.R. Wilk and S.D. Brown, "Modifications to the Simplex-Adapted Kalman Filter," Anal. Chim. Acta, 225, 37-53 (1989).

38.   T.Q. Barker and S.D. Brown, "Analysis of Partially Resolved Liquid Chromatographic Peaks by using Dynamic Modeling with the Kalman Filter," Anal. Chim. Acta, 225, 53-69 (1989).

39.   M. Redmond, H.R. Wilk and S.D. Brown, "Qualitative and Quantitative Analysis of Unresolved Responses in Liquid Chromatography with Fourier Transform Infrared Spectroscopic Detection," Anal. Lett., 22, 963-981 (1989).

40.   S.D. Brown, "Chemometrics: Fundamental Review," Anal. Chem., 62, 84R-101R (1990).

41.   S.D. Brown, "Real-Time Filtering of Data from Mobile, Passive Remote Infrared Sensors with Principal Component Models of Background," J. Chemometrics, 5, 147-161 (1991).

42.   S.D. Brown, "Rapid Parameter Estimation with Incomplete Chemical Calibration Models," Chemom. Int. Lab. Systems, 10, 87-105 (1991).

43.   R.J. Larivee and S.D. Brown, "Near-Optimal Smoothing of Noisy Data using a Maximum Entropy Criterion," Anal. Chem., 64, 2057-2066 (1992).

44.   S.L. Monfre and S.D. Brown, "Quantitative Fourier-Domain Analysis. Part 1: Analysis of Raw FTIR Interferograms," Applied Spectroscopy, 46, 1699-1710 (1992).

45.   S.L. Monfre and S.D. Brown, "Quantitative Fourier-Domain Analysis. Part 2: Determination of Boundary Conditions," Applied Spectroscopy, 46, 1711-1718 (1992).

46.   S. Sengupta, S. Cheeseman, S.D. Brown, and H. Foley, "Partial Least Squares Regression For Mass Spectral Analysis of H2 And D2 Scrambling Products," Industrial and Engineering Chemistry, 31, 2003-2010 (1992).

47.   S.D. Brown, R.S. Bear, Jr. and T.B. Blank, "Chemometrics: Fundamental Review," Anal. Chem., 64, 22R-49R (1992).

48. T.B. Blank and S.D. Brown, "Data Processing with Neural Networks," Anal. Chim. Acta, 277, 273-287 (1993).

49. R.S. Bear, Jr. and S.D. Brown, "Kalman Filter Optimized Simulation for Step Voltammetry," Anal. Chem., 65, 1061-1068, (1993).

50. R.S. Bear, Jr. and S.D. Brown, "Ultrasonic Pulse Method with Non-linear Calibration for Quantitative Monitoring of Polymer Blends Over a Wide Temperature Range," Anal. Chem., 65, 1169-1173, (1993).

51. T.B. Blank and S.D. Brown, "Nonlinear Multivariate Mapping of Chemical Data Using Feed-Forward Neural Networks," Anal. Chem., 65, 3081-3089 (1993).

52. S.D. Brown and R.S. Bear, Jr. "Chemometric Techniques in Electrochemistry: A Critical Review," CRC Crit. Rev. Analyt. Chem., 24, 99-131 (1993).

53. T.B. Blank and S.D. Brown, "Adaptive, Global Extended Kalman Filters for Training Feed-Forward Neural Networks," J. Chemometrics, 8, 391-408 (1994).

54. S.D. Brown, T.B. Blank, S.T. Sum and L.G. Weyer, "Chemometrics: Fundamental Review," Anal. Chem., 66, 315R-359R (1994).

55. T.B. Blank, S.D. Brown, A. Calhoun and D. Doren, "Neural Networks as Fitting Functions for Potential Energy Surfaces," J. Chem. Phys., 103, 4129-4137 (1995).

56. S.D. Brown, "Has the Chemometrics Revolution Ended?", Chemom. Intell. Lab. Syst., 30, 49-58 (1995).

57. S.D. Brown, "Chemical Systems Under Indirect Observation, Latent Properties and Chemometrics," Appl. Spectrosc., 49, 14A-31A (1995).

58. S.D. Brown, S.T. Sum, F. Despagne and B.K. Lavine, "Chemometrics: Fundamental Review," Anal. Chem., 68, 21R-61R (1996).

59. T.B. Blank, S.T. Sum, S.D. Brown and S.L. Monfre, "Transfer of Near-Infrared Calibrations Without Standards", Anal. Chem., 68, 2987-2995 (1996).

60. L.G. Weyer and S.D. Brown, "Application of New Variable Selection Techniques to Near Infrared Spectrometry," Journal of NIR Spectrometry, 4, 163-174 (1996).

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80.   S.D. Brown, "Time-Series Methods," In S.D. Brown, R. Tauler and B. Walczak, Eds. *Comprehensive Chemometrics*, 2nd Ed., Elsevier Scientific, Oxford, UK, 2020. Pages 371-398. https://doi.org/10.1016/B978-0-12-409547-2.14587-1

81.   S.D. Brown, "Data and Model Fusion Methods," In S.D. Brown, R. Tauler and B. Walczak, Eds. In *Comprehensive Chemometrics*, 2nd Ed., Elsevier Scientific, Oxford, UK, 2020. Chapter 3.16, Pages 317-339. https://doi.org/10.1016/B978-0-12-409547-2.14586-X.

82.   S.D. Brown, R. Tauler and B. Walczak, Eds. *Comprehensive Chemometrics*, 2nd Ed. Elsevier: Oxford, UK, 2020, hardcopy ISBN: 9780444641656.

STUDENTS GRADUATED

1.   Charles M. Phillips (M.S., 1980, University of California, Berkeley).
Non-thesis degree.
Presently Staff Scientist, Laser Facility, University of Pennsylvania.

2.   Brian C. Raine (M.S., 1981; University of California, Berkeley).
Non-thesis degree
Presently on technical sales staff, Hewlett-Packard Co., San Jose, CA.

3.   Jeffrey J. Toman (Ph.D., 1982, University of California, Berkeley).
Thesis Title: Convolution Techniques in Analytical Electrochemistry.
Presently on the research staff, Chevron Research, Albany, CA.

4.   Teri A. Floyd (Ph.D., 1982, University of California, Berkeley, University of Washington (joint)). Thesis Title: Metal Speciation Studies Using Electrochemical and Parameter Estimation Techniques.
Presently Principal, Floyd-Snider Consulting, Seattle, WA.

5.   Sarah C. Rutan (M.S., 1983; Ph.D., 1984, Washington State University).
Thesis Title: Pulsed Photoacoustic Spectroscopy and Digital Filtering for Studies of Metal Speciation.
Presently Professor, Virginia Commonwealth University, Richmond, VA.

6.   Donna M. Caster (M.S., 1983; Ph.D., 1985, Washington State University).
Thesis Title: Application of Digital Methods of the Study of Voltammetric Reactions.
Presently Manager, Astra-Zeneca Pharmaceuticals, Wilmington, DE.

7.   Caroline A. Scolari (M.S., 1984; Ph.D., 1986, Washington State University).
Thesis Title: Application of Digital Methods to Flow Injection Analysis.
Presently on the research staff, BioRad, Albany, CA.

8.   Molly Redmond Lockmeyer (M.S., 1988, University of Delaware).
Thesis Title: Multicomponent Analysis of Mixtures by LCIR with Kalman Filtering.
Presently on the research staff, Oxychem, Houston TX.

9.   Harlan L. Wilk (Ph.D., 1989, University of Delaware)
Thesis Title: Novel Methods for Adaptive Kalman Filtering
Presently on the research staff, Goodyear, Inc., Akron, OH.

10.   Robert J. Larivee (Ph.D., 1989, University of Delaware)
Thesis Title: New Methods of Factor Analysis
Presently Professor and Chairman, Frostburg State University, Frostburg, MD.

11.   Todd Q. Barker (Ph.D., 1991, University of Delaware)
Thesis Title: Analysis of Transient Chemical Species in Analytical Chemistry using the Kalman Filter. Presently Manager of Quality Assurance, Robbins, Pleasanton, CA.

12.   Steven J. Stuart (B.S. (Honors) 1990, University of Delaware)

Thesis Title: Application of Fuzzy Set Theory to Curve Fitting

Presently Professor of Chemistry, Clemson University, Clemson, SC.

13.   Stephen L. Monfre (Ph.D., 1992, University of Delaware)

Thesis Title: Kalman Filtering in Alternate Domains

Presently COO, Feather-Sensors, LLC, Princeton, NJ.

14.   Robert S. Bear, Jr. (Ph.D., 1994, University of Delaware)

Thesis Title: Simulation and Modeling in Step Voltammetry

Presently Manager of Research, Ametek, Inc., Pittsburgh, PA.

15.   Lois G. Weyer. (Ph.D., 1996, University of Delaware)

Thesis Title: Chemometric Methods Applied to the Near-Infrared and Raman Analysis of Water-Alcohol-Acetone Mixtures. Retired, 2013.

16.   Thomas B. Blank (Ph.D., 1996, University of Delaware)

Thesis Title: Multivariate Analysis of Chemical Data Using Multilayer Perceptrons

Presently on the research staff, C8MediSensors, San Jose, CA.

17.   Stephen T. Sum (Ph.D., 1998, University of Delaware)

Thesis Title: Multivariate Instrument Standardization

Presently Vice President for Research, InfraredX, Cambridge, MA

18.   Catherine Savage (M.A., 2000, University of Delaware). Non-thesis degree.

Presently employed as Forensic Chemist, Houston City Prosecutor's Office.

19.   Kristen Mello Rigg (M.S., 2002, University of Delaware)

Thesis Title: Novel "Hybrid" Classification Method Employing Bayesian Networks.

Not presently employed in chemistry.

20.   Nathaniel A. Woody (Ph.D., 2004, University of Delaware) Thesis Title: Novel Techniques for Data Mining and Pattern Recognition.   Presently on the research staff, Pfizer Pharmaceuticals, Groton, CT

21   Chun Wu (Ph.D., 2005, University of Delaware). Thesis Title: Nucleation and Growth of An Amyloidogenic Hexapeptide (NFGAIL) in Aqueous Solution Observed in Molecular Dynamics Simulations. Presently Assistant Professor, Rowan University, Glassboro, NJ.

22   Anthony J. Myles (Ph.D., 2005, University of Delaware) Thesis Title: An Investigation of Chemical Pattern Recognition Methodologies. Presently Vice President, core programming, quantitative finance, J.P. Morgan, Newark, DE.

23   Robert Feudale, (Ph.D., 2005, University of Delaware) Thesis Title: Novel Approaches to Multivariate Signal Preprocessing and Target Detection. Presently Assistant Professor, Camden County College.

24   Jalice Manso, (MS, 2008, University of Delaware) Thesis Title: Sensor Fusion of IR, NIR and Raman Spectroscopic Data for Polymorph Quantitation of an Agrochemical Compound. Presently on the research staff, DuPont de Nemours, Newark, DE.

25.   Wangdong Ni (Ph.D. 2010, South Central University, Changsha, China). Thesis Title: "Novel approaches to mutivariate calibration and classification and calibration maintenance" (Ru-Lin Man, co-advisor). Presently process engineer, Sembcorp Industries Ltd, Singapore.

26.   Stephen Kaster, (M.S, 2013) Thesis Title: "Data fusion with Parafac and Transfer of Stacked Local Classifiers." Presently research chemist, QS Pharma, Boothwyn, PA.

27.   Liyuan Chen, (Ph.D., 2014). Thesis Title: "Geospatial Pattern Recognition: Geographical Pattern Knowledge Discovered From Surface Water Data." Presently employed in quantitative finance, Wilmington, DE.

28.   Yushan Liu, (Ph.D., 2014). Thesis Title: "Dealing With Missing Data: Imputation For Multivariate, Finite Mixture Data." Presently research chemometrician, Atlanta, GA.

29.	Katie Daisey, (Ph.D., 2017). Thesis Title: "Examining Geospatial Data by use of Hierarchical, Multi-label Classification." Presently research chemometrician, Arkema, Inc, King of Prussia, PA.
30.	Dominic Poerio (Ph.D., 2018). Thesis title: "Localization Approaches to Increase Robustness in Spectral and Process Data Models With Diverse Applications." Presently Data Scientist, Axalta Inc., Philadelphia, PA.
31.	Casey Kneale (Ph.D., 2018) Thesis title: "Chemometric Investigations with Minimal Suppositions." Presently research data scientist, Kaiser Optical, Ann Arbor , MI.

INVITED TALKS

1.	"Trace Metal Analysis and Speciation", Department of Environmental and Earth Sciences, University of California, Riverside, CA, Feb., 1979.
2.	"Kinetic Effects in Voltammetric Determination of Metal Complex Stability Constants", Department of Civil Engineering, University of Washington, Seattle, WA, March, 1979.
3.	"Actinide Methods for Determining Trace Metal Partitioning and Speciation", West Coast Water Chemistry Winter Conference, USGS, Menlo Park, CA, December, 1980.
4.	"Analytical Methods for Determining Trace Metal Partitioning and Speciation", West Coast Water Chemistry Winter Conference, USGS, Menlo Park, CA, December, 1980.
5.	"Trace Metal Speciation in Environmental Samples", Department of Environmental and Health Sciences, University of California, Berkeley, April, 1980.
6.	"Convolution Voltammetry Applied to Questions of Metal Speciation", General Chemistry Division, Lawrence Livermore Laboratory, CA, April, 1980.
7.	"Novel Applications of Computers to Electrochemistry", Analytical Chemistry Division, Dow Chemical Company, Midland, MI, August, 1980.
8.	"Metal Speciation by Computer-Controlled Electrochemistry", Department of Chemistry, Oregon State University, Corvallis, OR, November, 1980.
9.	"Metal Speciation by Computer-Controlled Electrochemistry", Chemistry Department, Cornell University, Ithaca, NY, December, 1980.
10.	"Metal Speciation by Computer-Controlled Electrochemistry", Chemistry Department, Washington State University, Pullman, WA. December, 1980.
11.	"Chemical Speciation: Approaches Using Computer-Controlled Voltammetry", Department of Chemistry, University of California, CA, January, 1981.
12.	"Chemical Speciation: Approaches Using Computer-Controlled Voltammetry", Department of Chemistry, Oregon Graduate Center, Portland, OR, February, 1981.
13.	"Peak Deconvolution Using the Kalman Filter", Department of Chemistry, Portland State University, Portland, OR, February, 1981.
14.	"Resolution of Overlapped Electrochemical Peaks Using the Kalman Filter", 181st National Meeting of the ACS., Atlanta, GA, March, 1981.
15.	"Speciation of Labile and Quasi-Labile Metal Complex Systems Using the Kalman Filter", DOE/NBS Workshop on Environmental Speciation and Monitoring Needs for Trace Metal-Containing Substances from Energy-Related Processes, National Bureau of Standards, Gaithersburg, MD, May, 1981.
16.	"Speciation of Labile and Quasi-Labile Metal Complex Systems Using the Kalman Filter", Argonne National Laboratory, Argonne, IL, May, 1981.

17.   "Application of Computers to Electrochemistry: Two Methods of Electrochemical Peak Deconvolution", Department of Chemistry, University of Idaho, Moscow, ID, September, 1981.
18.   "Numerical Evaluation of Electrochemical Convolution Integrals Using Transform Techniques", 185th National Meeting of the ACS, Seattle, WA, March 1983.
19.   "Multicomponent Analysis by Flow Injection and Rapid-Scan Voltammetry",186th National Meeting of the ACS, Washington, DC., September, 1983.
20.   "Multicomponent Analyses by Flow Injection", Department of Chemistry, University of Idaho, Moscow, ID, October, 1983.
21.   "Adaptive Kalman Filtering", Department of Chemistry, University of Washington, Seattle, WA, February, 1985.
22.   "The Adaptive Kalman Filter in Multicomponent Analysis", Pittsburgh Conference on Analytical Chemistry, New Orleans, LA, February, 1985.
23.   "Pulsed Photoacoustic Spectroscopy and Digital Filtering", Department of Physics, University of Idaho, Moscow, ID, April, 1985.
24.   "Adaptive Kalman Filtering", NBS Conference on Chemometrics, Gaithersburg, MD, May, 1985.
25.   "Some Applications of Kalman Filtering in Electrochemistry", Virginia Commonwealth University, Department of Chemistry, May, 1985.
26.   "Kalman Filtering in Electrochemistry", Department of Chemistry, University of Delaware, July, 1985.
27.   "Peak Resolution Methods", Gordon Conference on Analytical Chemistry, New Hampton School, NH, August, 1985.
28.   "Applications of Kalman Filtering Methods", Electrochemical Society National Meeting, Las Vegas, NV, October, 1985.
29.   "The Kalman Filter in Dynamic Systems", FACSS, Philadelphia, PA, September, 1985.
30.   "Real-Time Analysis Using the Kalman Filter", ORNL-DOE Conference on Analytical Chemistry in Energy Technology, Knoxville, TN, October, 1985.
31.   "Signal Processing Methods", Eastern Analytical Symposium, New York, NY, November, 1985.
32.   "The Kalman Filter in Chemical Kinetics", Dept. of Chemistry, Reed College, Portland, OR, November, 1985.
33.   "The Kalman Filter in Analytical Chemistry: A New Approach for Solving Some Old Problems", 191st National Meeting of the ACS, New York, NY, April, 1986.
34.   "Data Reduction and Chemical Modeling with Digital Filters", 191st National Meeting of the ACS, New York, NY, 1986.
35.   "The Future of Instrumentation-Contained Chemometric Software", International Meeting of the Association for Clinical Chemistry, Chicago, IL, 1986.
36.   "Chemometrics as Analytical Instrumentation", ARCO Symposium on New Instrumental Techniques in Analytical Chemistry, ARCO Chemical Company, Newtown Square, PA, September 1986.
37.   "Adaptive Kalman Filtering for Multicomponent Chemical Analysis", Department of Statistics, University of Illinois, Urbana, IL, October, 1986.
38.   "New Uses of Adaptive Kalman Filters", Eastern Analytical Symposium, New York, NY, October, 1986.
39.   "Some Analytical Applications of Digital Filters", Department of Chemistry, Duke University, Durham, NC, October, 1986.
40.   "Kalman Filtering in Computer-Controlled Electrochemistry", Scientific Computing and Automation Conference, Atlantic City, NJ, November, 1986.

41.   "Kalman Filtering of Chemical Kinetics", Department of Chemistry, Purdue University, West Lafayette, IN, November, 1986.

42.   "Chemical Measurement and Data Reduction from a Systems Analysis Perspective", Pittsburgh Conference on Analytical Chemistry, Atlantic City, NJ, March, 1987.

43.   "Digital Filters in Multicomponent Chemical Analysis", E.I. DuPont Co., Wilmington, DE, July, 1987.

44.   "Digital Filters for Kinetic Analysis in Flow Systems", Eastern Analytical Symposium, New York, NY, September, 1987.

45.   "Multicomponent Analysis in Static and Flow Solution", NBS Conference on Trace Analysis, Gaithersburg, MD, September, 1987.

46.   "New Approaches in Kinetic Analysis", Seton Hall University, E. Orange, NJ, October, 1987.

47.   "Optimization of Digital Simulations using the Extended Kalman Filter", Scientific Computing Conference, Atlantic City, NJ, November, 1987.

48.   "Multicomponent Analysis without Separations", Eastman Kodak Co., Rochester, NY, December, 1987.

49.   "Real-Time Multicomponent Analysis using the Kalman Filter", CAC88, Amsterdam, The Netherlands, May, 1988.

50.   "Digital Filtering for Chemical Analysis and Modeling", Technical University of Vienna, Vienna, Austria, June, 1988.

51.   "Real-Time Chemical Analysis of Transient Samples using Digital Filtering Methods", Technical University of Graz, Graz, Austria, June, 1988.

52.   "Curve Resolution and Purity Determination of Poorly Resolved Chromatographic Peaks Using Kalman Filtering", 12th International Symposium on Column Liquid Chromatography, Washington, DC, June, 1988.

53.   "Real-Time Analysis of Mixtures using Digital Filters", Department of Chemistry, Villanova, PA, September, 1988.

54.   "Robust Adaptive Filtering of Infrared Spectra for Real-Time Multicomponent Analysis", Eastern Analytical Symposium, New York, NY, October, 1988.

55.   "Real-Time Multicomponent Analysis using the Kalman Filter", FACSS Conference, Boston, MA, October, 1988.

56.   "Getting Something for Nothing: Mixture Analysis using Digital Filters", Mobil Research and Development Corporation, October, 1988.

57.   "Real-Time Multicomponent Analysis using the Kalman Filter", Princeton Applied Research Corp., Princeton, NJ, November, 1988.

58.   "Real-Time Signal Processing of Complex Mixtures," U.S. Army CRDEC, Aberdeen Proving Ground, MD, September, 1989.

59.   "Characterization of Mixtures using Factor Analysis and Minimum Entropy", FACSS Conference, Chicago, IL, October, 1989.

60.   "Rapid Parameter Estimation using Incomplete Calibration Models," Mathematics In Chemistry Conference, College Station, TX, November, 1989.

61.   "Chemometric Methods for Qualitative and Quantitative Analysis of Complex Mixtures," University of Maryland, College Park, MD, November, 1989.

62.   "Applications of Chemometric Methods in Analytical Chemistry," Hercules Chemical Co., Wilmington, DE, November, 1989.

63.   "Getting Something for Nothing: Analytical Chemistry in the Absence of Information," Pennsylvania State University, University Park, PA, December, 1989.

64.   "Real-Time Signal Processing of Infrared Emission Data," Pittsburgh Conference on Analytical Chemistry and Spectroscopy, New York, NY, March, 1990.

65.   "Analytical Chemistry in the Absence of Prior Information", University of Alaska, Anchorage, AK, March, 1990.

66.   Tensorial Calibration (Invited Discussant), Gordon Conference on Mathematics and Statistics in Chemistry and Chemical Engineering, New Hampton School, NH, July, 1990.

67.   "Qualitative and Semi-quantitative Analysis of Poorly-Defined Mixtures", SCA Conference, Philadelphia, PA, September, 1990.

68.   " Digital Filtering with Incomplete Signal Information", FACSS Conference, Cleveland, OH, October, 1990.

69.   "Qualitative and Semi-quantitative Analysis of Poorly-Defined Mixtures", Lebanon Valley College, Annville, PA, October, 1990.

70.   "Applications of Digital Filtering," EPA Conference on Chemometrics and Statistics, Las Vegas, NV, November, 1990.

71.   " Digital Filtering with Incomplete Signal Information", Alcoa Aluminum Company, Pittsburgh, PA , November, 1990.

72.   " Digital Filtering with Incomplete Signal Information", DuPont Company, Wilmington, DE, November, 1990.

73.   "Qualitative and Semi-Quantitative Analysis of Poorly-Defined Mixtures", ATOChem North America, King of Prussia, PA, November, 1990.

74.   "Qualitative and Semi-Quantitative Analysis of Poorly-Defined Mixtures", ICI Pharmaceuticals, Wilmington, DE , December, 1990.

75.   "Real-Time Analysis of Passive Remote Infrared Data by Recursive Digital Filtering", Dickinson College, Carlisle, PA, February, 1991.

76.   "Getting Something for Nothing in Chemistry", SAS Lecture, Louisiana Section, New Orleans, LA, April, 1991.

77.   "Real-Time Analysis of Passive Remote Infrared Data by Recursive Digital Filtering", Emory University, Atlanta, GA, April, 1991.

78.   "Getting Something for Nothing in Chemistry", SAS Lecture, Piedmont Section, Atlanta, GA, April, 1991.

79.   "Qualitative and Semi-quantitative Analysis of Poorly-Defined Mixtures", Drexel University, Philadelphia, PA, May, 1991.

80.   "Neural Networks in Near-IR Analysis", Pittsburgh Conference on Analytical Chemistry and Spectroscopy, New Orleans, March, 1992.

81.   "Multivariate Processing of Pyrolysis-Mass Spectral Responses for Several Bacteria and Common Interferents", Snowbird Conference on Computer-Enhanced Spectroscopy, Snowbird, UT, June, 1992.

82.   "Data Processing with Neural Networks" Conference on Chemometrics in Analytical Chemistry (CAC-V), Montreal, Canada, July, 1992 (Plenary Lecture).

83.   "Fuzzy Kalman Filtering", Computer Applications in Analytical Chemistry (COMPANA), Jena, Germany, August, 1992 (Plenary Lecture).

84.   "Adaptive Kalman Filtering", FACSS, Philadelphia, PA, September, 1992.

85.   "Neural Networks for Chemical Calibration and Classification", FACSS, Philadelphia, PA, September, 1992.

86.   "On-line Ultrasonic Monitoring and Non-linear PLS Processing of Polymerization Reactions", FACSS, Philadelphia, PA, September, 1992.

87.   "Nonlinear Calibration with Neural Networks", Dept. of Chemistry, West Chester University, West Chester, PA, November, 1992.

88.   "Nonlinear Calibration and Classification with Neural Networks", DuPont Co., Wilmington, DE, February, 1993.

89.   "Calibration and Classification with Neural Networks", Dept. of Chemistry, Villanova University, Villanova, PA, April, 1993.

90.   "Nonlinear Calibration and Pattern Recognition with Backpropagation Neural Networks", Gordon Conference on Statistics in Chemistry and Chemical Engineering, New Hampton School, New Hampton, NH, July, 1993.

91.   "Nonlinear Calibration and Pattern Recognition with Neural Networks Optimized with Adaptive, Quasi-Newton Optimizers", NIST, November, 1993.

92.   "Nonlinear Calibration and Pattern Recognition with Neural Networks Optimized with Adaptive, Quasi-Newton Optimizers", E.I. duPont Neural Networks Resource Center, Wilmington, DE, December, 1993.

93.   "Classification and Calibration with Feedforward Neural Networks", Gesellshaft der Österreicher Chemiker, Vienna, Austria, January, 1994.

94.   "Some Remarks on the Training and Use of Neural Networks for Classification and Regression", Snowbird Conference on Computer-Enhanced Analytical Spectrometry, June, 1994.

95.   "It's Not Magic: It's Chemometrics", Dept. of Chemistry, Dalhousie University, Halifax, NS., Canada, June, 1994.

96.   "It's Not Magic: It's Chemometrics", Sun Oil Co., Marcus Hook, PA, June, 1994.

97.   "Is the Chemometrics Revolution Dead? Some Thoughts on the History and Future of Chemometrics", 1st INCINC Conference, WWW, September-November, 1994. (Plenary lecture.)

98.   "Nonlinear Multivariate Calibration and Modeling with Neural Networks", Eastern Analytical Symposium, Somerset, NJ, November, 1994.

99.   "Interfacial Methods for Studying Interfacial Reactions", Gordon Research Conference on Electrochemistry, Ventura, CA, January, 1995

100.   "Adaptive Neural Nets and Their Relatives", Symposium on the Future of Analytical Chemistry, Pittsburgh Conference, New Orleans, LA, March, 1995.

101.   "Chemometrics", Symposium on Analytical Chemistry, Royal Society of Chemistry, Hull, England, July, 1995. (plenary lecture)

102.   "Nonlinear and Weighted Principal Components Analysis," Gordon Research Conference on Statistics in Chemistry and Chemical Engineering, New Hampton, NH, August, 1995.

103.   " Nonlinear Multivariate Calibration and Modeling with Neural Networks", Pennsylvania State University, State College, PA, November, 1995.

104.   "Transfer of Calibrations in Solid-Phase NIR Spectroscopy," EAS, Somerset, NJ, November, 1995.

105.   "A Tutorial on Chemometric Methods for Process Control," ATOChem, Groupement Analytique NA,   King of Prussia, PA, April, 1996.

106.   "Transfer of Multivariate Calibrations without Standards", CPAC Semi-Annual Sponsors Meeting, Seattle, WA, May, 1996

107.   "Transfer of Multivariate Calibrations without Standards", DuPont Experimental Station, Wilmington, DE, June, 1996.

108.   "Transfer of Multivariate Calibration", Southern Illinois University, Carbondale, IL, September, 1996.

109.   "Transfer of Multivariate Calibrations Between Instruments", Dow Chemical ASQG Address, Midland, MI, September, 1996.

110.   "Transfer of Multivariate Calibrations Between Instruments," DuPont Symposium on Experimental Design and Modeling, Wilmington, DE, November, 1996.

111.   "Robust Calibration and Calibration Transfer in UV-Visible Spectroscopy," EAS, Somerset, NJ, November, 1996.

112.   "Some Applications of Digital Filtering," EAS, Somerset, NJ, November, 1996. (Award address).

113.   "Transfer of Calibrations in NIR, " Seventh International Conference on Near Infrared Spectroscopy, Essen, Germany, September, 1997 (Plenary lecture).

114.   "Making Chemometrics Work: Transfer of Multivariate Calibrations," University of Delaware, September, 1997. (Colloquium)

115.   "Transfer of Calibration," NIST, Gathersburg, MD, December, 1997.

116.   "Data Analysis in Chemistry and Chemical Engineering," NSF-NIST Vision2020 Panel Presentation, New Orleans, LA, March, 1998.

117.   "Transfer of Calibration," Allied Signal Co., Morristown, NJ, May, 1998.

118.   "Transfer of Calibration," Chambersburg Meeting on NIR Spectroscopy, Chambersburg, PA, August, 1998.

119.   "Calibration Transfer," SmithKline Beecham Symposium on Analytical Chemistry, October, 1998.

120.   "Transfer of Multivariate Calibration," Vrije Universiteit Brussel, Farmaceutisches Instituut, November, 1998.

121.   "CART, ACE, MARS, PPR, and Neural Networks: What's the Difference Anyway?" Annual Meeting of the Belgian Chemometrics Society, Teurven, Belgium, November, 1998.

122.   "Standardization of Instruments and Spectra in Multivariate Calibration," Annual Meting of the Belgian Chemometrics Society, Teurven, Belgium, November, 1998.

123.   "Enhanced Classification with Bayesian Networks and Recursive Partitioning," Symposium on Computational Chemistry, Pfizer Central Research, Groton, CT, January, 1999.

124.   "Hybrid Bayes Networks for Classification," FACCSS Kowalski Retirement Symposium, Vancouver, BC, October, 1999.

125.   "Hybrid Bayes Networks for Classification," DuPont CRD, Wilmington, DE, January, 2000.

126.   "Hybrid Bayes Networks for Classification," ASA Symposium on Novel Methods in Statistics, Newark, DE, 2000.

127.   "Novel Calibration Methods for Process Chemical Data," Bayer Diagnostics, Elkhart, IN, September 2000.

128.   "Hybrid Bayes Networks for Classification of QSAR and Process Chemical Data," International Conference on Chemometrics and Environmetrics, Las Vegas, NV, October, 2000.

129.   "Novel Calibration Techniques for Spectroscopic Data", Bayer GMBH, Levercruzen, Germany, July, 2001. (Plenary lecture)

130.   "Believe it or Not! New Methods Employing Bayes Theorem in Calibration and Classification," EAS Conference, Atlantic City, NJ, October, 2001.

131.   Data, Information and Knowledge and the Role of Soft Modeling, ECU Distinguished Professorship Lecture, East Carolina University, September, 2001. (Plenary lecture)

132.   "Transfer of Calibrations and Robust Analyses," IFPAC Conference, San Diego, CA, January, 2002 (Invited Main Speaker)

133.   "Wavelet Multiscale Regression Analysis for Multivariate Calibration, " 8th Conference on Chemometrics in Analytical Chemistry, Seattle, WA, September, 2002 (Plenary lecture)

134.   "Improved Piecewise Orthogonal Signal Correction," 8th Conference on Chemometrics in Analytical Chemistry, Seattle, WA, September, 2002.

135.   "The use of Continuous and Discrete Variables for Regression and Classification in Bayesian Networks," 8th Conference on Chemometrics in Analytical Chemistry, Seattle, WA, September, 2002.

135.   "Transferring and Improving the Robustness of Multivariate Calibrations," ACS National Meeting, Boston, MA, September, 2002.

136. "Dual Domain PLS Regression," EAS Conference, Somerset, NJ, November, 2003.

137. Multiscale Methods for Calibration, Classification and Calibration Transfer, IFPAC Conference, Arlington, VA, January, 2004.

138. H.B. White,III, S.D. Brown and M.V. Johnston, "Contemporary Moral Problems in Chemistry: Impact of Peer Presentations on Awareness of Science and Society Issues," ACS National Meeting, Anaheim, CA, 2004. (H. White presented)

139. "Chemometrics in Process Analytical Technology ", Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, April, 2004.

140. "Chemometric Methods for PAT" Bristol-Myers-Squibb, Princeton, NJ, August, 2004.

141. "Novel Approaches to Classification for Use with High-Dimensional Data, Chemometrics in Analytical Chemistry (Plenary lecture), Lisbon, Portugal, September, 2004.

142. "Chemometrics in Process Analytical Technology," Astra Zeneca, Wilmington, DE, December, 2004.

143. "Chemometrics in Process Analytical Technology: Making Useful Models Interpretable and Interpretable Models Useful," US Food and Drug Administration, Rockville, MD, December, 2004.

144. "Resolution of Poorly Characterized Mixtures with Chemometrics," ICI Symposium, Strongsville, OH, June, 2005.

145. "Chemometrics Applications in Homeland Security", Centra Corporation, Arlington, VA, July, 2005.

146. "Chemometrics in Metabolomics", Invited Discussant, Gordon Research Conference, South Hadley, MA, 2005.

147. "Chemometrics in Process Analytical Technology," NIST-NIH CARB Conference on PAT, Rockville, MD, Dec. 2005

148. "Fusion of Data and Models in Classification and Regression," International Chemometrics Research Meeting (ICRM), Veldhoven, Netherlands, June, 2006.

149. "Fusion of Data and Models in Classification and Regression," Exxon Research and Engineering, Annandale, NJ, June, 2006.

150. "Fusion of Data and Models in Classification and Regression," CAC-2006 Conference (Plenary Lecture), Aguas de Lindoia, Brazil, September, 2006.

151. "Fusion of Models for Regression and Classification," EAS Conference, Somerset, NJ, November, 2006

152. "Glucose Analysis in vitro and in vivo," University of Missouri, Columbia, MO, April, 2008. (Colloquium)

153. "Glucose Analysis in vitro and in vivo," State University of New York, Buffalo, NY, September 2008. (SAS Tour)

154. "Multivariate Fusion of Data and its Application in Process Calibration," EAS Symposium, November, 2008.

155. "Wavelet OSC and Stacked methods for Classification ," FACSS Conference, Louisville, KY, October, 2009.

156. "Getting the Most from a Partial Least Squares Calibration," FACSS Conference , Louisville, KY, October 2009.

157. "Data Fusion for Analysis of Pharmaceutical Systems," FACSS Conference , Raleigh, NC, October 2010.

158. "Calibration and Classification Transfer using Stacked Methods," FACSS Conference, Raleigh, NC, October 2010.

159. "Fusing NIR and other Spectra for Quality Assurance of Pharmaceuticals," Eastern Analytical Symposium, Somerset, NJ, November, 2010.

160.   "Estimating Class Uncertainties in Geospatial Classification of Surface Water," NGA-NARP Conference, Washington, DC, August, 2011. (Winner, Best Presentation of Conference)

161.   "Classification Uncertainty Estimates" ICRM Conference, Nijmegen, Netherlands, September, 2011.

162.   "What's to be Gained by Combining Multiple Sets of Measurements?", FACSS Conference, Reno, NV, October 2011.

163.   "What's Missing? Dealing with the Consequences of Incomplete Data," EAS Conference, Somerset, NJ, November, 2011.

164.   "Wavelet Transforms for Multivariate Calibration and Classification", Irstea, Montpellier, France, March, 2012.

165.   "Transfer of Multivariate Calibrations," Ondalys, Montpellier, France, April, 2012.

166.   "Stacked Methods in Calibration and Classification," Irstea, Montpellier, France, May, 2012.

167.   "Data Fusion in Chemometrics," Irstea, Montpellier, France, July, 2012.

168.   "Bayesian Regression: Is it Worth the Trouble?" SciX (FACSS) Conference, Kansas City, MO, October 2012.

169.   "Geospatial Data Mining: Estimating Location and Uncertainty from Multivariate Geospatial Data," EAS Conference, Somerset, NJ, November, 2012.

170.   "Estimating Class Uncertainties in Multivariate Geospatial Data," NARP-NURI Conference, Washington, DC, August, 2012. (L. Chen presented)

171.   "Imputing Left-censored Data and Estimating Class Uncertainties from Multivariate Geospatial Data," NARP-NURI Conference, Washington, DC, September 11, 2013 (Yushan Liu presented).

172.   "Estimating Class Uncertainties in Multivariate Geospatial Data," (Success Story Presentation) NARP-NURI Conference, Washington, DC, September 11, 2013.

173.   "Determining Location of Surface Water Samples by Analysis of the Chemical Signature," NARP-NURI Conference, Washington, DC, September 11, 2013 (Liyuan Chen presented).

174.   "Geospatial Data Mining: Uncertainties in Clustering and Classification of Multivariate Geochemical Data,"SciX Conference, Milwaukee, WI, October 1, 2013.

175.   "Ascertaining Uncertainty in Hierarchical, Tree-Structured Models," IC-Academic Research Symposium, Washington, DC, September 15, 2015.

176.   "Issues in Hierarchical Modeling of Complex Data," SciX Conference, Providence, RI, September 29, 2015.

177.   "The Corporate Approach in Chemometrics: Using a Hierarchy in Classification of Complex Data," EAS Conference, Somerset, NJ, Nov. 17, 2015.

178.   "Policy Issues in Modeling Data with a Hierarchy," 251st ACS National Meeting, San Diego, CA, March 3, 2016 (Katie Daisey presented).

179.   "Variable Selection for Calibration", 252nd ACS National Meeting, Philadelphia, PA, August 22, 2016 (Cannon Giglio presented).

180.   "An Elastic Variable Selection Approach to Calibration", SciX Conference, Minneapolis, MN, September 22, 2016.

181.   "Selecting and Incorporating Hierarchy in Classification", ICARS Conference, Washington, DC, September 23, 2016. (Katie Daisey presented).

182.   "Stacking the Deck in Calibration: Better Models and Better Transfers with Stacked Calibration Methods," Eastern Analytical Symposium, Princeton, NJ, November, 2017.

183.   "The Dao of Bruce: How Kowalski Shaped the Early Days of Chemometrics", 17th Conference on Chemometrics in Analytical Chemistry (CAC-2018), Halifax, NS, Canada, June 25, 2018. (Plenary Address)

184. "Calibration Transfer Without Transfer Standards", SciX Conference, Atlanta, GA, October 24, 2018.

185. "Partial Least Squares Methods for Variable Selection, Predictions in the Presence of Uncalibrated Interferents, and Calibration Transfer," SciX Conference, Atlanta, GA, October 24, 2018.

186. "Some Perspectives on the History and Sociology of the Chemometrics Revolution" (Invited Plenary Presentation), Chimometrie 2019, Montpellier, France, January 29, 2019. (Plenary Address)

CONTRIBUTED TALKS

1.   "Chemistry of Chromyl Fluoride," NW. Regional ACS Conference, Corvallis, OR, 1972.

2.   "Chemical Properties of Chromyl Fluoride and Chromium Pentafluoride", Seventh International Fluorine Chemistry Conference, Santa Cruz, CA, 1974.

3.   "Laboratory Interfaces for the PDP-11 Minicomputer", NW. Regional ACS Conference, Portland, OR, 1977.

4.   "Computer-Controlled Voltammetry: Sensitivity and Response Factors", Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, Cleveland, OH, 1978.

5.   "Pseudopolarography: Theory and Application to the Determination of Metal Complex Stability Constants", First Symposium on Environmental Analytical Chemistry, Provo, UT, 1978.

6.   "Evaluation of the Impact of Coal Mining on Water Quality by Pattern Recognition", First Symposium on Environmental Analytical Chemistry, Provo, UT, 1978.

7.   "Determination of the Stability Constants for the CdClx System by Convolution Potential Sweep Voltammetry", West Coast Water Chemistry Winter Conference, Stanford University, Palo Alto, CA, 1979.

8.   "Electrochemical Determination of Stability Constants in Natural Waters: The Kalman Filter", West Coast Water Chemistry Winter Conference, Stanford, CA, 1980.

9.   "Computer-Controlled Convolution Sweep Voltammetry", Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, Atlantic City, NJ, 1981.

10.   "Noise Structure Effects in the Reduction of Electrochemical Data", Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, Atlantic City, NJ, 1981.

11.   "Trace Determination and Complexation of Nd(III) in Aqueous Solution by Laser-Induced Photoacoustic Spectroscopy", Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, Atlantic City, NJ, 1981.

12.   "Trace Metal Speciation Using the Kalman Filter", NW Regional ACS Conference, Eugene, OR, 1982.

13.   "Novel Uses of Computers in Chemistry: Electroanalytical Methods Using the Computer", Linfield College, McMinnville, OR, 1982.

14.   "Speciation of Quasilable Metal Complex Systems Using Adaptive Digital Filtering", 185th National ACS Meeting, Seattle, WA, 1983.

15.   "Determination of Heterogeneous Kinetic Parameters Using Digital Simulation and the Kalman Filter", 185th National ACS Meeting, Seattle, WA, 1983.

16.   "Use of Pulsed Voltammetric Techniques Combined with Digital Filtering for Study of Metal-Liquid Complexation", 185th National Meeting of the ACS, Seattle, WA, 1983.

17.   "Multicomponent Analysis Using Square-Wave Voltammetry with a Digital Filter", 185th National Meeting of the ACS, Seattle, WA, 1983.

18.   "Pulsed Photoacoustic Spectroscopy of Metal Species in Solution", 185th National Meeting of the ACS, Seattle, WA, 1983.

19.   "In Situ Pulsed Photoacoustic Spectroscopy for Selective Determination of Sorbed and Solution Praseodymium Species", NW Regional ACS Conference, Honolulu, HI, 1983.

20.   "Microcomputers in Chemical Analysis: The State of the Art and Some Future Trends", NW Regional ACS Conference, Moscow, ID, 1984.

21.   "Multicomponent Analysis by Flow Injection and Rapid-Scan Voltammetry", NW Regional ACS Conference, Moscow, ID, 1984.

22.   "Application of the Extended Kalman Filter to the Study of Metal Complexation Kinetics", NW Regional ACS Conference, Moscow, ID, 1984.

23.   "Digital Filtering Methods in Electrochemistry and Photoacoustic Spectroscopy", Department of Chemistry, Reed College, Portland, OR, 1984.

24.   "Digital Filtering Methods in Electrochemistry and Photoacoustic Spectroscopy", Department of Chemistry, Portland State University, Portland, OR, 1984.

25.   "Digital Filtering Methods in Electrochemistry and Photoacoustic Spectroscopy", Department of Chemistry, Linfield College, McMinnville, OR,1984.

26.   "Application of Digital Methods to the Study of Pulsed Voltammetric Responses of Kinetic Systems", Pittsburgh Conference on Analytical Chemistry, New Orleans, LA, 1985.

27.   "Multicomponent Analysis by Flow Injection and Rapid-Scan Voltammetry", Pittsburgh Conference on Analytical Chemistry, New Orleans, LA, 1985.

28.   "Depletion Effects in Normal Pulse Voltammetry: Studies Using Digital Simulation and Kalman Filtering", Pittsburgh Conference on Analytical Chemistry, Atlantic City, NJ, 1986.

29.   "Applications of Rapid-Scan Square-Wave Voltammetric Detection in Flow Injection Analysis", Pittsburgh Conference on Analytical Chemistry, Atlantic City, NJ, 1986.

30.   "Kalman Filtering of Flow Injection Data", NW Regional ACS Conference, Portland, OR, June, 1986.

31.   "Factor Analysis of Chemically Interacting Mixtures", Mid-Atlantic Regional ACS Conference, Baltimore, MD, September, 1986.

32.   "Analysis of Transient Species Concentration in Flowing Streams", Mid-Atlantic Regional ACS Conference, Baltimore, MD, September, 1986.

33.   "Analysis of Reaction Kinetics using FTIR and the Kalman Filter", Mid-Atlantic Regional ACS Conference, Baltimore, MD, September, 1986.

34.   "Background and Solvent Removal in LC-ATR-FTIR using Adaptive Filtering", Mid-Atlantic Regional ACS Conference, Baltimore, MD, September, 1986.

35.   "Multicomponent HPLC Analysis using an Adaptive Kalman Filter", Pittsburgh Conference on Analytical Chemistry, Atlantic City, NJ, March, 1987.

36.   "Multicomponent Analysis using Diffuse Reflectance", Pittsburgh Conference on Analytical Chemistry, Atlantic City, NJ, March 1987.

37.   "Parameter Estimation of Chemical Kinetic Data using the Extended Kalman Filter", Pittsburgh Conference on Analytical Chemistry, Atlantic City, NJ, March, 1987.

38.   "Multicomponent Analysis of Liquid Phase IR Spectra using the Kalman Filter", Pittsburgh Conference on Analytical Chemistry, Atlantic City, NJ, March, 1987.

39.   "Digital Filtering in Flow Solution", National Meeting of the ACS, New Orleans, LA, September, 1987.

40.   "Kalman Filtering in Alternate Domains", FACSS, Detroit, MI, October, 1987.

41.   "Examination of Complex Equilibria using Kalman Filtering and Minimum Entropy", Pittsburgh Conference on Analytical Chemistry, New Orleans, LA, February, 1988.

42.   "Multicomponent Analysis using Fuzzy Set Theory and the Kalman Filter", Pittsburgh Conference on Analytical Chemistry, New Orleans, LA, February, 1988.

43.   "HPLC Curve Resolution and Peak Purity Determination using the Kalman Filter and Photodiode Array Detection", Pittsburgh Conference on Analytical Chemistry, New Orleans, LA, February,1988.

44.   "Kalman Filtering in Alternate Domains", Pittsburgh Conference on Analytical Chemistry, New Orleans, LA, February, 1988.

45.   "Real-Time Chemical Analysis using the Kalman Filter", Pittsburgh Conference on Analytical Chemistry, New Orleans, LA, February, 1988.

46.   "Improved Adaptive Kalman Filters", Pittsburgh Conference on Analytical Chemistry, New Orleans, LA, February, 1988.

47.   "Fuzzy Calibration", Mid-Atlantic Regional Analytical Chemistry Conference, Potsdam, NY, October, 1988.

48.   "Real-Time Chromatographic Analysis using Recursive Digital Filtering", Pittsburgh Conference on Analytical Chemistry, Atlanta, GA, March, 1989.

49.   "Parameter Estimation in the Fourier Domain", Pittsburgh Conference on Analytical Chemistry, Atlanta, GA, March, 1989.

50.   "Optimal Fourier Smoothing of Spectra using Minimum Entropy", Pittsburgh Conference on Analytical Chemistry, Atlanta, GA, March, 1989.

51.   "A Robust, Adaptive Kalman Filter for Real-Time Analysis", Pittsburgh Conference on Analytical Chemistry, Atlanta, GA, March, 1989.

52.   "Nonlinear Calibration" (Poster), Pittsburgh Conference on Analytical Chemistry, Atlanta, GA, March, 1989.

53.   "Knocking the Rough Edges off Data with Entropy," Mid-Atlantic Regional Analytical Chemistry Conference, Villanova, PA, October, 1989.

54.   "Optimizing Digital Simulations of Voltammetry with Recursive Digital Filters", MARM, Newark, DE, May, 1991.

55.   "Teaching Chemometrics to Undergraduates", ACS National Meeting, New York, NY, August, 1991.

56.   "Investigation of Systematic Errors in Electrochemical Simulations", FACSS, Philadelphia, PA, September, 1992.

57.   "Modeling Nonlinear Data with Neural Networks, MARM, Fairfax, VA, December, 1992.

58.   "Interfacial Studies of Interfacial Reactions," University of Delaware Colloquium, May, 1993.

59.   "Classification and Detection with Feedforward Neural Networks," Scientific Conference on Chemical Defense Research, Edgewood, MD, November, 1993.

60.   "Some Practical Considerations in Using Neural Nets for Nonlinear Modeling," Eastern Analytical Symposium, November, 1993.

61.   "Determination of Bacterial Mixtures in Soil Bioremediation", Scientific Conference on Chemical Defense Research, Edgewood, MD, November, 1995.

62.   "Transfer of Multivariate Calibrations without Standards", Mid-Atlantic Regional ACS Meeting (MARM), Villanova, PA, May, 1996.

63.   "Robust Calibration," EAS Conference, Somerset, NJ, November 1997.

64.   "Wavelets and background removal in Multivariate calibration," Gordon Research Conference, Plymouth, NH, 1997 (poster presentation).

65.   "Bayesian Nets and Classification," EAS Conference, Somerset, NJ, 1998.

66.   "Wavelet Methods for Multivariate Calibration," EAS Conference, Somerset, NJ, 1998.

67.   "Combining Recursive Partitioning and Uncertain Reasoning for Data Exploration and Characteristic Prediction ," AAAI Symposium on Predictive Toxicology, Stanford, CA, March, 1999.

68. "Calibration Transfer with Wavelets," EAS, Atlantic City, NJ, October, 2000.
69. "Standard-Free Calibration Transfer of NIR Spectra," EAS, Atlantic City, NJ, October 2001.
70. "Wavelet Multiscale Calibration of Spectroscopic Data," EAS, Atlantic City, NJ, October 2001. (Winner of EAS Poster Talk Award)
71. "Fuzzifying Classification Trees for Improved Prediction," CAC-8, Seattle, WA, September 2002 (poster)
72. "Novel Methods for Transfer and Strengthening Multivariate Calibrations," CPAC Conference, Seattle, WA, May 2003.
73. "Data Mining and Classification," CPAC Conference, Seattle, WA, May 2003.
74. "Application of Partial Least Squares Regression to the Automatic Detection of Chemical Vapors by Passive Infrared Remotely Sensed Image Data, SPIE Conference, Providence, RI, October, 2003. (Poster talk)
75. "Combining Predictive Modeling Techniques," Eastern Analytical Symposium, Somerset, NJ, November, 2003.
76. "Dual-Domain Calibration Transfer for Spectral Data," Eastern Analytical Symposium, Somerset, NJ, November, 2003.
77. "Automatic Detection of Chemical Vapors by Passive Infrared Remotely Sensed Image Data Using Partial Least Squares Regression," Eastern Analytical Symposium, Somerset, NJ, November, 2003.
78. "Frequency-Domain Discrimination: A New Classification Technique for Spectral Data," Eastern Analytical Symposium, Somerset, NJ, November, 2003.
79. "Novel Methods for Transfer and Strengthening Multivariate Calibrations," CPAC Conference, Seattle, WA, May 2004.
80. "Data Mining and Classification," CPAC Conference, Seattle, WA, May 2004.
81. "Novel Methods for Transfer and Strengthening Multivariate Calibrations," CPAC Conference, Seattle, WA, November, 2004.
82. "Data Mining and Classification," CPAC Conference, Seattle, WA, November, 2004.
83. "Novel Methods for Transfer and Strengthening Multivariate Calibrations," CPAC Conference, Seattle, WA, May, 2005.
84. "Data Mining and Classification," CPAC Conference, Seattle, WA, May, 2005.
85. "Novel Methods for Transfer and Strengthening Multivariate Calibrations," CPAC Conference, Seattle, WA, November, 2005.
86. "Data Mining and Classification," CPAC Conference, Seattle, WA, November, 2005.
87. "Novel Methods for Transfer and Strengthening Multivariate Calibrations," CPAC Conference, Seattle, WA, May, 2006.
88. "Data Mining and Classification," CPAC Conference, Seattle, WA, May, 2006.
89. "Novel Methods for Transfer and Strengthening Multivariate Calibrations," CPAC Conference, Seattle, WA, November, 2006.
90. "Data Mining and Classification," CPAC Conference, Seattle, WA, November, 2006.
91. "Novel Methods for Transfer and Strengthening Multivariate Calibrations," CPAC Conference, Seattle, WA, May, 2007.
92. "Data Mining and Classification," CPAC Conference, Seattle, WA, May, 2007.
93. "Novel Methods for Transfer and Strengthening Multivariate Calibrations," CPAC Conference, Seattle, WA, November, 2007.
94. "Data Mining and Classification," CPAC Conference, Seattle, WA, November, 2007.
95. "Identifying Biomarkers of the MHC Gene to Investigate Chemosensory Discrimination", (poster presentation), UMBC Undergraduate Research Symposium, October, 2007. (1st place Award in Biology Division to Tyler Bazzoli)

96. "Identifying Biomarkers of the MHC Gene to Investigate Chemosensory Discrimination", UD HHMI Undergraduate Research Symposium, April, 2008, presented by Tyler Bazzoli)

97 "Glucose Analysis in vitro and in vivo," University of Delaware, Newark, DE, September, 2008. (Colloquium)

98. "Identifying Biomarkers of the MHC Gene to Investigate Chemosensory Discrimination", (poster presentation), UMBC Undergraduate Research Symposium, October, 2008. (Earned 1st place Award in Chemistry Division to Tyler Bazzoli)

99. "Improving Robustness of Calibration Models by Signal Processing and Stacking Methods", CPAC Conference, Seattle, WA, November, 2008. (Wandong Ni presented)

100. "Chemometric Methods for Biomarker Discovery," Freshman Poster Session, University of Delaware, December 8, 2009. (with T. Bazzoli)

101. "Chemometric Methods for Biomarker Discovery," Freshman Poster Session, University of Delaware, December 8, 2010. (with T. Bazzoli)

102. "Multivariate Calibration by Bayesian Regression on PLS scores and on selected variables," ICNIRS Conference, la Grande Motte, France, June 3, 2013 (with J.-M. Roger)

103. "Imputing left-censored multivariate environmental data for cluster analysis and classification," EAS Conference, Somerset, NJ, November 16, 2013 (with Yushan Liu).

104. "Determining Location of Surface water samples by analysis of the chemical signature," EAS Conference, Somerset, NJ, November 16, 2013 (with Liyuan Chen).

105. "Outer Product Analysis (OPA) For Calibration Transfer," (poster presentation) Summer Scholars Undergraduate Research Symposium, Newark, DE, August 13, 2015 (with Cannon Giglio)

106. "Outer Product Analysis (OPA) For Calibration Transfer," (poster presentation) Undergraduate Research Symposium in the Chemical and Biological Sciences, Baltimore, MD, October 3, 2015 (with Cannon Giglio) (winner, 1st Place poster).

107. "Variable Selection with an Elastic Net," (poster presentation) Summer Scholars Undergraduate Research Symposium, Newark, DE, August 11, 2016 (with Cannon Giglio).

108. "Variable Selection with an Elastic Net," (poster presentation) Eastern Analytical Symposium, Somerset, NJ, November 15, 2016 (EAS Award to Cannon Giglio).

109. "Selection of Meaningful Spectral Variables with an Elastic Net," (poster presentation) Chemometrics in Analytical Chemistry, Halifax, NS, June 26, 2018. (Cannon Giglio presented)

SESSIONS CHAIRED AND ORGANIZED

1. Session Chair, Division of Analytical Chemistry, NW Regional ACS Conference, Eugene, OR, 1982.

2. Session Chair, Division of Analytical Chemistry, 185th National ACS Conference, Seattle, WA, 1983.

3. Session Chair, NATO Advanced Studies Institute on Chemometrics, Cosenza, Italy, 1983.

4. Divisional Organizer, NW Regional ACS Conference, Moscow, ID, 1984.

5. Divisional Organizer, NW Regional ACS Conference, Portland, OR, 1986.

6. Program Committee and Divisional Organizer, Scientific Computing and Automation, Atlantic City, NJ, 1986.

7. Session Organizer, Eastern Analytical Symposium, New York, NY, 1986.

8. Session Organizer, Eastern Analytical Symposium, New York, NY, 1987.

9.   Program Committee and Divisional Organizer, Scientific Computing and Automation, Atlantic City, NJ, 1987.

10.   Conference Organizer, Middle Atlantic Regional Academic Analytical Chemistry Conference, Newark, DE, 1987.

11.   Session Organizer, National Meeting of the ACS, Miami, FL, September, 1989.

12.   Session Organizer, Conference on Mathematics in Chemistry, College Station, TX, November, 1989.

13.   Section Leader (Chemometrics) , Gordon Research Conference, New Hampton School, NH, August, 1990.

14.   Program Committee, Scientific Computing and Automation Conference, September,1990.

15.   Session Organizer and Session Chair, FACSS Conference, Cleveland, OH, October, 1990.

16.   Program Committee, Chemometrics in Analytical Chemistry V, Montreal, Quebec, July, 1992.

17.   Program Committee and Session Chair, COMPANA 1992: Computer Applications in Analytical Chemistry, Jena, Germany, August,1992.

18.   Poster Chairman, FACSS Conference, Philadelphia, PA, September,1992.

19.   Session Organizer and Session Chair, American Statistical Association National Meeting, San Francisco, August, 1993.

20.   Conference Chair, Snowbird Conference on Computer-Enhanced Analytical Spectrometry, Snowbird, UT, June,1994.

21.   Program Committee, European Conference on Chemometrics, Vals, The Netherlands, July, 1994.

22.   Organizing Committee, INCINC Computer Network Conference on Chemometrics, September-December, 1994.

23.   Organizing Committee, Conference on Mathematics and Statistics in Chemistry, Las Vegas, NV, 1995.

24.   Session Organizer and Session Chair, EAS Conference, Somerset NJ, 1996.

25.   Session Organizer and Chair, Chemometrics Award Symposium, EAS Conference, Somerset, NJ, 1997.

26.   Session Organizer and Chair, Kowalski Award Symposium, FACSS, Vancouver, BC, October, 1999.

27.   Session Chair and Program Committee, CAC-8, Seattle, WA, September, 2002.

28.   Session Organizer and Chair, EAS Conference, Somerset, NJ, November, 2003.

29.   Session Organizer and Chair, ACS National Conference, Philadelphia, PA, July, 2004.

30.   Session Chair, Chemometrics in Analytical Chemistry Conference, Lisbon, Portugal, September, 2004.

31.   Session Chair, EAS Conference, Somerset, NJ, November, 2004.

32.   Session Chair, NIH-NIST Conference on Process Analytical Technology, Rockville, MD, December, 2005.

33.   Program Committee, CAC-10, Campinas-Lindoia, Brazil, September, 2006.

34.   Program Committee, International Conference on Near Infra-Red Spectroscopy 2013, La Grande Motte, France, June, 2013.

35.   Program Committee, Chemometrics in Analytical Chemistry, Richmond, VA, June, 2014.

36.   Session Organizer and Chair, 252nd ACS National Meeting, Philadelphia, PA, August, 2016.

37.   Session Organizer and Chair, Eastern Analytical Symposium, Princeton, NJ , November, 2017.

38.   Session Chair, 17th Conference on Chemometrics in Analytical Chemistry (CAC-2018), Halifax, NS, Canada, June 26, 2018