BIOGRAPHICAL SKETCH

Provide the following information for the key personnel in the order listed for Form Page 2.
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NAME	POSITION TITLE
Hettich, Robert L.	Distinguished Research Scientist

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, and include postdoctoral training.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	YEAR(s)	FIELD OF STUDY
South Dakota School of Mines and Technology, Rapid City, South Dakota	B.S.	1982	Chemistry
Purdue University, West Lafayette, Indiana	Ph.D.	1986	Analytical Chemistry

A. Positions and Honors:

Positions and Employment

1980-1982 Research Assistant, Experiment Station, South Dakota School of Mines and Technology, Rapid City, SD
1986-2009 Research staff scientist, Oak Ridge National Laboratory
2009 - Distinguished research scientist, Oak Ridge National Laboratory
2000- Adjunct faculty member, University of Tennessee, Genome Sciences Graduate School
2011- Joint faculty member, University of Tennessee, Microbiology Department
2014- Faculty member, Bredesen Center for Interdisciplinary Research/ Graduate Education.

Other Experience and Professional Memberships

1986 - American Society for Mass Spectrometry
1990-1996 ORISE Traveling Lecture Program
1996-1997 East Tennessee Mass Spectrometry Discussion Group, chairman
2000- Review member for NIH-NCI Study Sections on Quantitative Proteomics
2001- Dissertation advisor for ORNL-UTK Ph.D. graduate students
2002 - Review member for NIH General Medicine Study Sections
2002 Review member for NIH Study Section of High-End Instrumentation Grants
2004- Review member for NIH-NCI Study Section on IMAT
2004 Chairman, NIH Study Section for New Technologies for Metabolomics
2006 Chairman, NIH Study Section for Clinical Proteome Tech. for Cancer Research
2008 Chairman, NIH Study Section for Clinical Proteomics Applications
2008- Editorial Advisory Board, *Mass Spectrometry Reviews*
2010- Editorial Advisory Board, *BMC Genomics*
2016- Associate editor, *Microbiome*
2014 Session organizer for International Mass Spectrometry Conference (Geneva, Switzerland)
2019-2021 ASMS, Vice-president for arrangements

Honors

1993 Martin Marietta Energy Systems Technical Achievement Award
2018 ORNL Outstanding graduate student mentor award
2019 ORNL Distinguished Research Award

B. Peer-reviewed publications (in chronological order)

1. "Heteronuclear Transition Metal Cluster Ions in the Gas Phase: Photodissociation and Reactivity of VFe^+," R.L. Hettich and B.S. Freiser, J. Amer. Chem. Soc., (1985), 107, 6222.

2. "Photodissociation of $FeCH_2^+$ and $CoCH_2^+$: Determination of the Carbene, Carbyne, and Carbide Bond Strengths," R.L. Hettich and B.S. Freiser, J. Amer. Chem. Soc., (1986) 108, 2537.

3. "Gas Phase Photodissociation of Organometallic Ions: Bond Energy and Structural Determinations," R.L. Hettich, T.C. Jackson, E.M. Stanko, and B.S. Freiser, J. Amer. Chem. Soc., (1986) 108, 5086.

4. "Determination of Carbide, Carbyne, and Carbene Bond Energies by Gas Phase Photodissociation of $RhCH_2^+$, $NbCH_2^+$, and $LaCH_2^+$," R.L. Hettich and B.S. Freiser, J. Amer. Chem. Soc., (1987) 109, 3543.

5. "Spectroscopic and Thermodynamic Investigations of Transition Metal Cluster Ions in the Gas Phase: Photodissociation of MFe^+," R.L. Hettich and B.S. Freiser, J. Amer. Chem. Soc., (1987) 109, 3537.

6. "Gas Phase Photodissociation of Transition Metal Ion Complexes and Clusters," R.L. Hettich and B.S. Freiser, Fourier Transform Mass Spectrometry: Evolution, Innovation, and Applications, ACS Symposium Series 359, M.V. Buchanan, Editor, 1987.

7. "The Gas Phase Ion Chemistry of Methyl and Ethyl Borate," R.L Hettich, T. Cole, and B.S. Freiser, Inter. J. Mass Spectrom. Ion Proc., (1987) 81, 203.

8. "Ligand Effects on Transition Metal Ion Reactivity: Primary and Secondary Reactions of Co^+ and Ni^+ with Alkenes," R.L Hettich and B.S. Freiser, Organomet, (1989), 8, 2447.

9. "The Differentiation of Methyl Guanosine Isomers by Laser Ionization Fourier Transform Mass Spectrometry," R.L. Hettich, Biomed. Environ. Mass Spec., (1989) 18, 265.

10. "Characterization of Photo-induced Pyrimidine Cyclobutane Dimers by Laser Desorption Fourier Transform Mass Spectrometry" R. L. Hettich, M.V. Buchanan, and C.-h. Ho, Biomed. Environ. Mass Spec., (1990) 19, 55.

11. "Structural Investigations of Aluminum Cluster Ions, Al_n^- (n=3-50)," R. L. Hettich, J. Amer. Chem. Soc., (1989) 111, 8582.

12. "Investigation of UV Matrix-Assisted Laser Desorption Fourier Transform Mass Spectrometry for Peptides," R. L. Hettich and M. V. Buchanan, J. Amer. Soc. Mass Spec., (1991) 2, 22.

13. "Laser Ablation Studies of Palladium Electrolytically Loaded with Hydrogen and Deuterium," M. J Shea, R. N. Compton, and R. L. Hettich, Phys. Rev. A, (1990) 42, 3579.

14. "Structural Characterization of Normal and Modified Oligonucleotides by Matrix-Assisted Laser Desorption Fourier Transform Mass Spectrometry," R. L. Hettich and M. V. Buchanan, J. Amer. Soc Mass Spec. (1991), 2, 402.

15. "Matrix-Assisted Laser Desorption Fourier Transform Mass Spectrometry for Biological Compounds," Proceedings of the NATO Workshop on Methods and Mechanisms for Producing Ions from Large Molecules, edited by K. Standing and W. Ens, Plenum Press, New York, 1991, 247-255.

16. "Doubly-Charged Negative Ions of Carbon-60," R. L. Hettich, R. N. Compton, and R. H. Ritchie, Phys. Rev. Lett. (1991), 67, 1242.

17. "Matrix-Assisted Laser Desorption Fourier Transform Mass Spectrometry for the Structural Examination of Modified Nucleic Acid Constituents," R. L. Hettich and M. V. Buchanan, Int. J. Mass Spec. Ion Proc. (1991), 111, 365.

18. "Applications of Matrix-Assisted Laser Desorption FTMS for Biomolecules," R. L. Hettich and M. V. Buchanan, Lecture Notes in Physics, 389, Laser Ablation Mechanisms and Applications, J.C. Miller and R. F. Haglund, Jr., editors, Springer-Verlag Publishers, New York, NY 1991, p. 160.

19. "Ion-Molecule Reactions of Carbon Cluster Anions," R. L. Hettich, Lecture Notes in Physics, 389, Laser Ablation Mechanisms and Applications, J.C. Miller and R. F. Haglund, Jr., editors, Springer-Verlag Publishers, New York, NY 1991, p. 280.

20. "Doubly-Charged Negative Ions of Bucky Ball - C_{60}^{2-} ," R. L. Hettich, R. N. Compton, and R. H. Ritchie, Lecture Notes in Physics, 389, Laser Ablation Mechanisms and Applications, J.C. Miller and R. F. Haglund, Jr., editors, Springer-Verlag Publishers, New York, NY 1991, p. 285.

21. "Applications of Mass Spectrometry to DNA Sequencing," K. B. Jacobson, H. F. Arlinghaus, C. H. Chen, G. L. Glish, R. L. Hettich, M. V. Buchanan, and S. A. McLuckey, Genetic Analysis Tech. Appl., (1991), 8, 223.

22. "Contribution to the Isolation and Characterization of the Buckminsterfullerenes," M. Diack, R.L. Hettich, R.N. Compton, and G. Guiochon, Anal. Chem., (1992) 64, 2143.

23. "Characterization and Stability of Highly Fluorinated Fullerenes," A.A. Tuinman, P. Mukherjee, J.L. Adcock, R.L. Hettich, and R.N. Compton, J. Phys. Chem., (1992) 96, 7584.

24. "Fullerenes from the Geological Environment," P.R. Buseck, S. Tsipursky, and R.L. Hettich, Science, (1992) 257, 215.

25. "Methyl Guanine Isomer Distinction by Hydrogen/Deuterium Exchange using a Fourier Transform Mass Spectrometer," B.D. Nourse and R.L. Hettich, J. Amer. Soc. Mass Spec., (1993) 4, 296-305.

26. "Rapid Extraction and Structural Characterization of Biomolecules in Agarose Gels by Laser Desorption FTMS," J. C. Dunphy, K. L. Busch, R. L. Hettich, and M. V. Buchanan, Anal. Chem., (1993) 65, 1329-1335.

27. "Characterization of Large Biomolecules by FTMS", M.V. Buchanan and R.L. Hettich, Anal. Chem., (1993) 65, 245A-259A.

28. "Characterization of Underivatized Pterins by Laser Desorption Fourier Transform Mass

Spectrometry", K. Bruce Jacobson and Robert L. Hettich, Pteridines, (1993) 4, 72-75.

29. "Laser Ablation and Laser Desorption Techniques with Fourier Transform Mass Spectrometry", Robert Hettich and Changming Jin, invited book chapter for Principles and Applications of Laser Ablation, J.C. Miller, editor, Springer Series in Materials Science 28, Springer-Verlag Publishers, Berlin, (1994), p. 135-154.

30. "Matrix-Assisted Laser Desorption/Ionization Fourier Transform Mass Spectrometry of Oligodeoxyribonucleotides," E.A. Stemmler, R.L. Hettich, G.B. Hurst, and M.V. Buchanan, Rapid Comm. Mass Spec., (1993) 7, 828-826.

31. "Characterization and Identification of Radiation-Induced Products of Thymidine-3'-Monophosphate and Thymidylyl (3'->5') Thymidine by Laser Desorption Fourier Transform Mass Spectrometry," H. Yoshida and R. Hettich, Radiation Research, (1994) 139, 271-279.

32. "Synthesis and Characterization of Molybdenum Carbide Clusters: Mo_nC_{4n} (n=1-4)", C. Jin, R.E. Haufler, R.L. Hettich, R.N. Compton, A.A. Puretzky, and A.V. Dem'yanenko, Science, (1994) 263, 68-71.

33. "Characterization of Naturally-Occurring and Modified Fullerenes by Fourier Transform Mass Spectrometry," R. Hettich, C. Jin, R. Compton (Oak Ridge National Laboratory) and P. Buseck and S. Tsipursky (Arizona State University), American Institute of Physics Conference Proceedings (Laser Ablation: Mechanisms and Applications-II), Vol 288, J.C. Miller and D.B. Goehegan, Editors, AIP Press, New York, (1994), p. 94-99.

34. "Laser Desorption Fourier Transform Mass Spectrometry Studies of Modified Fullerenes," C. Jin, R. Hettich, and R. Compton, American Institute of Physics Conference Proceedings (Laser Ablation: Mechanisms and Applications-II), Vol 288, J.C. Miller and D.B. Goehegan, Editors, AIP Press, New York, (1994), p. 141-147.

35. "Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry for the Structural Characterization of Modified Oligonucleotides," G. Hurst, R. Hettich, and M. Buchanan (Oak Ridge National Laboratory) and E. Stemmler (Bowdoin College, Brunswick, ME), American Institute of Physics Conference Proceedings (Laser Ablation: Mechanisms and Applications-II), Vol 288, J.C. Miller and D.B. Goehegan, Editors, AIP Press, New York, (1994), p. 519-525.

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38. "The Structural Characterization of Polycyclic Aromatic Hydrocarbon Dihydrodiol Epoxide DNA

Adducts Using Matrix-Assisted Laser Desorption/Ionization Fourier Transform Mass Spectrometry," E.A. Stemmler, M.V. Buchanan, G.B. Hurst, and R.L. Hettich, Anal. Chem., (1994), 66, 1274-1285.

39. "Determination of the Electron Affinities of Fluorinated Fullerenes ($C_{60}F_{44,46}$, $C_{70}F_{52,54}$) by Fourier Transform Mass Spectrometry," R. Hettich, C. Jin, and R. Compton, Int. J. Mass Spec. Ion Proc (Special Issue on Fullerenes), (1994) 138, 263-274.

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41. "Attachment of Two Electrons to $C_{60}F_{46,48}$: Shape Resonances in Multiply Charged Anions," C. Jin, R. Hettich, R. Compton, A. Tuinman, Phys. Rev. Lett., (1994) 73, 2821.

42. "Ionic Properties of Hydrogenated and Fluorinated Fullerenes," R.L. Hettich, C. Jin, P.F. Britt, A.A. Tuinman, and R.N. Compton, Mat. Res. Soc. Symp. Proc. (1994) 349, 133.

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45. "Low Level Detection of Chemical Agent Simulants in Meat and Milk by Ion Trap Mass Spectrometry," M.V. Buchanan, R.L. Hettich, J.H. Xu, L.C. Waters, and A. Watson, J. Hazard. Mat., (1995) 42, 49.

46. "Structural Characterization of Underivatized Pteridines by Laser Desorption Fourier Transform Mass Spectrometry," R. L. Hettich and K. B. Jacobson, J. Mass Spec., (1995) 30, 872.

47. "The Analysis of Modified Oligonucleotides by Matrix-Assisted Laser Desorption/ Ionization Fourier Transform Mass Spectrometry," E.A. Stemmler, M.V. Buchanan, G.B. Hurst, and R.L. Hettich, Anal. Chem., (1995) 67, 2924.

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49. "Mass Spectrometry and Small-Angle X-Ray Scattering and Studies of Gamma-Irradiated $C_{60,}$" R.L. Hettich, S. Henderson, R.N. Compton, and G. Bakale, J. Phys. Chem., (1996) 100 5426.

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54. "Concerning Naturally-Occurring Fullerenes in Shungite," R.L. Hettich and P. R. Buseck, Carbon, (1996) 34, 685-687.

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57. "Synthesis of Doped Fullerene Clusters and Boron-Nitrogen Tubules Using Laser Ablation," Z.C. Ying, J.G. Zhu, R.N. Compton, L.F. Allard, Jr., R.L Hettich, R.E. Haufler, invited book chapter for *Nanostructured Materials: Clusters, Composites, and Thin Films*, M. Moskovits and V.M. Shalaev, editors, (1998).

58. "Endohedral Metallofullerenes," A. Lahamer, Z.C Ying, R.E. Haufler, R.L. Hettich, and, R.N. Compton, invited book chapter for *Advances in Metal and Semiconductor Clusters, Vol. IV*, M. Duncan, editor, JAI Press, (1998), pp. 179-203.

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60. "Investigation of the Fragmentation and Oxygen Reactivity of Endohedral Metallofullerenes M@C60," R. Hettich, A. Lahamer, and R. Compton, Int. J. Mass Spec. Ion Proc., (Freiser focus issue), (1999) 182/183, 335-348.

61. "Formation and Characterization of Iron-Oligonucleotide Complexes with MALDI-FTICR," R. Hettich, J. Amer Soc. Mass Spec. (Freiser focus issue), (1999), 10, 941-949.

62. "Spacer Length Effect on the PET Fluorescent Probe for Alkali Metal Ions," H.-F. Ji, R. Dabestani, G. M. Brown, and R.L. Hettich, Photochem. Photobiol. J., (1999) 69, 513-516.

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Matrix-Assisted Laser Desorption/Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry," R.L. Hettich, Int. J. Mass Spec., (2001) 204, 55-75.

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74. "New Technologies for Nutrition Research," Sharon Ross, Pothur Srinivas, Andrew Clifford, Stephen Lee, Martin, Philbert, and Robert Hettich, J. Nutrition, (2004), 134, 681-685.
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85. "Community proteomics identifies key activities in a natural microbial biofilm," Rachna Ram, Nathan VerBerkmoes, Michael Thelen, Gene Tyson, Brett Baker, Robert Blake II, Manesh Shah, Robert Hettich, and Jillian Banfield," Science, 2005, 308, 1915-1920.
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Academic Responsibilities as adjunct faculty member at the University of Tennessee - Knoxville

Dissertation Major Advisor - (completed degrees):

- **Dr. Joshua Sharp**, "Development of Hydroxyl Free Radical Chemistry for the Surface Mapping of Proteins," Ph.D. awarded October 2003. (*academic faculty member at Univ. of Mississippi*)
- **Dr. Tomoaki Uchiki**, "Structure-Function and Regulation of Ribonucleotide Reductase Inhibitor, Sml1," Ph.D. awarded December 2004. (*research staff position in Japan*)
- **Dr. Nathan VerBerkmoes**, " Mass Spectrometry-Based Proteomics for Studying Microbial Physiology from Isolates to Communities," Ph.D. awarded May 2005 (*academic faculty member at UT-El Paso*)
- **Dr. Heather Connelly**, "Integrated Computational and Experimental Platform for Characterizing Protein Isoforms and PTMs in Microbial Systems by Top-Down FT-ICR Mass Spectrometry," Ph.D. awarded August 2006. (*staff member at Hospira, North Carolina*)
- **Dr. Chongle Pan**, "An Integrated Experimental and Computational Approach to Proteomics: Scaling from High Resolution Qualitative Analysis to Quantitative Measurements with Confidence Evaluation," Ph.D. awarded December 2006 (*staff member at ORNL*)
- **Ms. Demet Ataman**, failed comprehensive exam twice; she chose to leave GST program.
- **Ms. Kanan Vyas**, "The Integration of Oxidative Surface Mapping and Molecular Dynamics Simulation Techniques as a Strategy for Studying Protein Conformational Change," M.S. awarded August 2006. (*employed at a biotech company in San Francisco area*)
- **Dr. Melissa Thompson,** "Integrating Mass Spectrometry Based Proteomics and Bioinformatics Technologies for the Molecular Level Characterization of *Shewanella Oneidensis* To Chromate Exposure," Ph.D. awarded November 2007. (*staff member at Pfizer, St. Louis, MO*)
- **Dr. Carlee McClintock, "**Development of an Electrochemical Technique for Oxidative Surface Mapping to Investigate Solution-Phase Protein Dynamics with High Performance Mass Spectrometry and Advanced Informatics," Ph.D. awarded Dec. 2009. (*staff position at Pain Consultants research clinic, Knoxville, TN*)
- **Dr. Brian Erickson**, "Integrating Mass Spectrometric and Computational Technologies for the Characterization of Extracellular Proteins in a Natural Microbial Community," Ph.D. awarded Oct. 2010 (*post-doc at Harvard Medical School*)
- **Dr. Andrew Dykstra**, "Advanced Techniques in Mass Spectrometry for Qualitative and Quantitative Protein Characterization," Ph.D. awarded May 2011 (*research staff member at Amgen, New Hampshire*)
- **Dr. Alison Russell,** "Characterization of the Human Host Gut Microbiome with an Integrated Genomics/Proteomics Approach," Ph.D. awarded Oct. 2011 (*post-doc at Harvard Medical School*)
- **Dr. Adriane Lochner**, "Proteomic characterization of the cellulolytic enzyme system expressed by the extremely thermophilic bacteria *Caldicellulosiruptor* spp.," Ph.D. awarded Mar. 2012 (Germany; *currently instructor at Univ. of Hamburg*)
- **Dr. Jacque Young**, "Functional Characterization of Microbial Symbiotic Associations by Metaproteomics," Ph.D. awarded Nov. 2012 (*post-doctoral position at Univ. of Penn*.)
- **Dr. Paul Abraham,** "Development and application of mass-spectrometry-based proteomics to generate and navigate the proteomes of the genus *Populus*," Ph.D. awarded April, 2013 (*staff position at ORNL*)
- **Dr. Rachel Adams**, " Development and integration of informatics tools for qualitative and quantitative characterization of proteomic datasets generated by tandem mass spectrometry, Ph.D. awarded May, 2013 (*informatics consultant*)

- **Mr. Adam Martin, "**Demonstration of a targeted proteome characterization approach for examining specific metabolic pathways in complex bacterial systems," M.S. awarded Dec. 2013 (*currently instructor at Maryville College*).
- **Dr. Ritin Sharma, "**Development of an experimental and computational platform for enhanced characterization of modified peptides and proteins in environmental proteomics," Ph.D. awarded April 2014 (*post-doc at Moffitt Cancer Center, Florida)*
- **Dr. Zhou Li**, "Quantitative Characterization of Proteins and Post-Translational Modifications in Complex Proteomes Using High-Resolution Mass Spectrometry-Based Proteomics," Ph.D. awarded April 2014 (*currently post-doc at ORNL*)
- **Dr. Xiaoxin Liu**, "Comparative Proteomics Reveals Core vs. Unique Molecular Signatures for Dissimilatory Metal Reducing Bacteria Grown with Various Electron Acceptors," Ph.D. awarded Aug. 2014 (*currently in nursing school*)
- **Dr. Weili Xiong, "**Characterizing Early-life Microbiome Functionality in Premature Infant Gut by a Metaproteomics Approach," Ph.D. awarded Nov. 2015. (*currently post-doc at FDA*)
- **Dr. Chen Qian, "**Development of MS-based proteomics approaches to examine metabolic pathways and protein:protein interactions in microbial systems," Ph.D. awarded July 2017. (*currently post-doc in Baltimore*)
- **Dr. Ramsunder (Sarvesh) Iyer, "**Bioinformatic and Experimental Approaches for Deeper Metaproteomic Characterization of Complex Environmental Samples," Ph.D. awarded August 2017. (*currently post-doc at Northwestern Univ.)*
- **Dr. Suresh Poudel**, "Proteome characterizations of microbial systems using MS-based experimental and informatics approaches to examine key metabolic pathways, proteins of unknown function, and phenotypic adaptation," awarded July 2018 (*currently post-doc at ORNL*)
- **Dr. Mallory Ladd**, " Development and application of an untargeted exometabolomics approach to identify biogeochemical hotspots of dissolved organic matter vulnerability in Arctic soils," awarded November 2018. (*intern position Naval Research lab, Wash. D.C.*).

Dissertation Major Advisor for following graduate students (current):

- Mr. Manuel Ivan Villalobos-Solis, graduate student in GST-Ph.D. program
- Mr. Alfredo Blakeley-Ruiz, graduate student in GST-Ph.D. program
- Mr. David Reeves, graduate student in the ORNL-UTK Bredesen program.
- Mr. Alex Cope, graduate student in GST-Ph.D. program.
- Ms. Payal Chirania, graduate student in GST-Ph.D. program.
- Ms. Samantha Peters, graduate student in GST-Ph.D. program.
- Mr. Him Shrestha, graduate student in GST-Ph.D. program.
- Mr. Matthew Keller, graduate student in GST-Ph.D. program.
- Ms. Manasa Appidi, graduate student in GST-Ph.D. program.

Academic teaching:

- I am the lead instructor for the GST-II (LS 521) class on Analytical Technologies, and teach 10 MS lectures each spring.
- Every other fall, I am the lead instructor for an advanced graduate level class (LS 695) on Biological Mass Spectrometry. (*this class has been held every other year for the past 12 years*)
- Every semester, I teach a mass spectrometry-based journal discussion class at ORNL.

Expertise Summary

Dr. Robert Hettich is a distinguished research scientist and leader of the Bioanalytical Mass Spectrometry Group of the Biosciences Division at Oak Ridge National Laboratory and a joint faculty member in the Microbiology Department at the University of Tennessee. He has over 34 years of experience in biological mass spectrometry, with a particular focus on high performance mass spectrometry. His research interests involve the development and application of advanced mass spectrometry technology for characterizing complex biological mixtures, such as

microbial and plant proteomes. His group has pioneered the technology of metaproteomics, which is the characterization of the extensive protein inventory in natural microbial communities. His work in this arena spans from environmental microbiology (i.e. microbial communities in soil and groundwater ecosystems) to bioenergy (engineering of microbial solubilization of cellulosic biomass to generate biofuels and bioproducts) and finally to the human microbiome (characterizing the microbial connections between human health and disease). His group is active in development of both experimental and computational informatic methodologies for proteome research. He has authored more than 275 publications (h-index = 67 Google Scholar), and is active in mentoring graduate students, as well as teaching analytical technology and advanced biological mass spectrometry classes. He is an associate editor for Microbiome, a member of the editorial advisory boards of Mass Spectrometry Reviews, BMC Genomics, and Journal of Integrated Omics, and is an active review member on several NIH review study sections, in particular for NIH-GM and NIH-NCI-IMAT.