

BIOGRAPHICAL SKETCH

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NAME		POSITION TITLE	
Hettich, Robert L.		Distinguished Research Scientist	
EDUCATION/TRAINING (<i>Begin with baccalaureate or other initial professional education, such as nursing, and include postdoctoral training.</i>)			
INSTITUTION AND LOCATION	DEGREE (<i>if applicable</i>)	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 member, 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
 1987 - East Tennessee Mass Spectrometry Discussion Group, member
 1990-1996 ORISE Traveling Lecture Program
 1993-1997 Executive board member, Southern Appalachian Science and Engineering Fair
 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 Study Section on NCR
 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
 2007 Chairman, NIH Study Section for Biomedical Sensors
 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)

Honors

1994 Martin Marietta Energy Systems Technical Achievement 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.

Principal Investigator/Program Director (Last, First, Middle): _____

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 - C₆₀²⁻," 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.

Principal Investigator/Program Director (Last, First, Middle): _____

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. Goehagan, 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. Goehagan, 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. Goehagan, Editors, AIP Press, New York, (1994), p. 519-525.
36. "Laser Ablation of Graphite in Different Buffer Gases," A.A. Puretzky, D.B. Goehagan, R.E. Haufler, R.L. Hettich, X.-Y. Zheng, and R.N. Compton, American Institute of Physics Conference Proceedings (Laser Ablation: Mechanisms and Applications-II), Vol 288, J.C. Miller and D.B. Goehagan, Editors, AIP Press, New York, (1994), p. 365-374.
37. "Characterization of Modified Nucleic Acid Constituents by Matrix-Assisted Laser Desorption Mass Spectrometry," R. Hettich, G. Hurst, M. Buchanan, and E. Stemmler, Polycyclic Aromatic Compounds, M. Zander, editor, (1994) 6, 95-102.(peer-reviewed).

Principal Investigator/Program Director (Last, First, Middle): _____

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.
40. "Direct Solid Phase Hydrogenation of Fullerenes," C. Jin, R. Hettich, R. Compton, D. Joyce, J. Blencoe, and T. Burch, J. Phys. Chem., (1994), 98, 4215-4217.
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.
43. "Thermodynamic Characterization of the Plastic Crystal and Non-Plastic Crystal Phases of C_{70} ," Y. Jin, A. Xenopoulos, J. Cheng, W. Chen. B. Wunderlich, M. Diack, C. Jin, R.L. Hettich, R.N. Compton, and G. Guiochon, Mol. Cryst. Liq. Cryst., (1994) 257, 235-250.
44. "Production and Characterization of Metallofullerene Superatoms," Z.C. Ying, C. Jin, R.L. Hettich, A.A. Puretzky, R.E. Haufler, and R.N. Compton, in *Fullerenes: Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials*, edited by K.M. Kadish and R.S. Ruoff, (The Electrochemical Society, Pennington), 1995, Volume 94-24, p. 1402. (invited paper).
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.
48. "A New Interface for Combining Electrospray with Fourier Transform Ion Cyclotron Resonance Mass Spectrometry," L. Tang, R.L. Hettich, and M.V. Buchanan, Rapid Comm. Mass Spec., (1995) 9, 731.
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.
50. "Structural Determination and Ionic Properties of Endohedral Lanthanum Fullerenes," R.L. Hettich, Z. C. Ying, and R.N. Compton, *Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials: Volume 3*, K.M. Kadish and R.S. Ruoff, editors, The Electrochemical Society: Pennington, N.J. (1994), p. 1457.

Principal Investigator/Program Director (Last, First, Middle): _____

51. "Instability of Fullerene Molecules at a High Temperature," Z.C. Ying, R.N. Compton, B.A. DiCamillo, R.L. Hettich, and G.A. Guiochon, J. Phys. Chem., in press.
52. "Enrichment and Characterization of a Noble-Gas Fullerene: Ar@C₆₀," B.A. DiCamillo, R.N. Compton, R.L. Hettich, A.A. Tuinman, J. Cross, Jimenez-Vazquez, M. Saunders, J. Phys Chem., (1996) 100, 9197-9201.
53. "Investigation of Oligonucleotide Fragmentation with MALDI-FTMS and Sustained Off-Resonance Irradiation (SORI)," Robert Hettich and Elizabeth Stemmler, Rapid Comm. Mass Spec. (Special ORNL issue), (1996) 10 321.
54. "Concerning Naturally-Occurring Fullerenes in Shungite," R.L. Hettich and P. R. Buseck, Carbon, (1996) 34, 685-687.
55. "Synthesis of Nitrogen-Doped Fullerenes by Laser Ablation," Z.C. Ying, R.L. Hettich, R.N. Compton, and R.E. Haufler, J. Phys. B, (1996) 29, 4935-4942.
56. "Sonochemical Synthesis of C₆₀H₂," D. Mandrus, M. Kele, R.L. Hettich, G. Guiochon, B.C. Sales, and L.A. Boatner, J. Phys. Chem., (1997) 101, 123-128.
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.
59. "Cadiolides A and B, New Metabolites from an Ascidian of the Genus *Botryllus*," C.J. Smith, R.L. Hettich, J. Jompa, A. Tahir, M.V. Buchanan, and C. M. Ireland, J. Org. Chem., (1998), 63, 4147-4150.
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.
63. "Optical Sensing of Cesium Using 1,3-Alternate Calix[4]-mono- and di(anthrylmethyl)-aza-crown-6," Ji, H F, Dabestani R, Hettich R L, Brown G M, Photochemistry and Photobiology (1999) 70 882-886.
64. "Investigating the Effect of Transition Metal Ion Oxidation State on Oligodeoxyribonucleotide Binding by Matrix-Assisted Laser Desorption/Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry," R.L. Hettich, Int. J. Mass Spec., (2001) 204, 55-75.

65. "Characterization of Monomeric and Dimeric Forms of Recombinant *Sml1p-histag* Protein by Electrospray-MS," T. Uchiki, R. Hettich, V. Gupta, and C. Dealwis, *Anal. Biochem.*, (2002) 301, 35-48.
66. "Synthesis and sensing behavior of cyanoanthracene modified 1,3-alternate calix[4]benzocrown-6: a new class of Cs⁺ selective optical sensors," Ji HF, Dabestani R, Brown GM, Hettich RL, *Journal of the Chemical Society-Perkin Transactions*, 2 (4): 585-591 APR 2001.
67. "N-Phenyl-1,4-Phenylenediamine and Benzidine Oxidation Products Identified Using On-Line Electrochemistry/Electrospray Fourier Transform Mass Spectrometry," V. Kertesz, H. Deng, K.G. Asano, R.L. Hettich, and G.J. Van Berkel, *Electroanalysis*, (2002), 14, 1027-1030.
68. "Intact Protein Analysis for Site Directed Mutagenesis Overexpression Products: Plasmid Encoded R67 Dihydrofolate Reductase," N.C. VerBerkmoes, M.B. Strader, D. Smiley, E.E. Howell, G.B. Hurst, R. L. Hettich, and J.L. Stephenson, Jr., *Anal. Biochem.*, (2002), 305, 68-81.
69. "Integrating "Top-Down" and "Bottom-Up" Mass Spectrometric Approaches for Proteomic Analysis of *Shewanella oneidensis*," N.C. VerBerkmoes, J.L. Bundy, L. Hauser, K.G. Asano, J. Razumovskaya, F. Larimer, R.L. Hettich, and J.L. Stephenson, Jr., *J. Proteome Research*, (2002), 1, 239-252.
70. "Protein Surface Mapping by Chemical Oxidation: Structural Analysis by Mass Spectrometry," J. Sharp, J. Becker, and R.L. Hettich, *Anal. Biochem.* (2003), 313, 216-225.
71. "Mass Spectrometry", Nathan VerBerkmoes, Joshua Sharp, and Robert Hettich, in *Microbial Functional Genomics*, edited by Jizhong Zhou, Dorothea Thompson, Ying Xu, and James Tiedje, John Wiley & Sons, New Jersey, 2004, pp. 241-282.
72. "Comparison of Sustained Off-Resonance Irradiation Collisionally Activated Dissociation and Multipole Storage-Assisted Dissociation for Top-Down Protein Analysis," Karin Keller, Jennifer Brodbelt, Robert Hettich, and Gary Van Berkel, *J. Mass Spec.* (2004), 39, 402-411.
73. "Identification of Phosphorylation Sites on the Yeast Ribonucleotide Reductase Inhibitor Sml1," T. Uchiki, R. Hettich, and C. Dealwis *J. Biol. Chem.* (2004), 279, 11293-11303.
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.
75. "Sml1p is a Dimer in Solution: Characterization of Denaturation and Renaturation of Recombinant Sml1p," Vibha Gupta, Cynthia Peterson, Lezlee Dice, Tomoaki Uchiki, Joseph Racca, Jun-tao Guo, Ying Xu, Robert Hettich, Xiaolan Zhao, Rodney Rothstein, and Chris Dealwis, *Biochemistry*, (2004), 43, 8568-8578.
76. "A Computational Method for Assessing Peptide-Identification Reliability in Tandem Mass Spectrometry Analysis with Sequest," Jane Razumovskaya, Victor Olman, Dong Xu, Ed Uberbacher, Nathan VerBerkmoes, Robert Hettich, and Ying Xu," *Proteomics*, (2004), 4, 961-969.
77. "Analysis of Protein Solvent Accessible Surfaces by Photochemical Oxidation and Mass Spectrometry," J. Sharp, J. Becker, and R.L. Hettich, *Anal. Chem.* (2004), 76, 672-683.
78. "Mass Spectrometric Approaches for Characterizing Bacterial Proteomes," Nathan VerBerkmoes, Heather Connelly, Chongle Pan, and Robert Hettich, *Expert Review in Proteomics*, (2004), 1, 433-447.
79. "Characterization of the 70S Ribosome from *Rhodospseudomonas palustris* Using an Integrated "Top-Down" and "Bottom-Up" Mass Spectrometric Approach," Strader M, VerBerkmoes N, Tabb D, Connelly H, Barton J, Bruce B, Pelletier D, Davison B, Hettich RL, Larimer F, Hurst G., *J Proteome Res.*, (2004), 3, 965-978.
80. "A Graph-Theoretic Approach to Separation of b and y Ions in Tandem Mass Spectra," Bo Yan, Chongle Pan, Victor Olman, Robert Hettich, and Ying Xu, *Bioinformatics*, (2005), 21, 563-574.
81. "Transcriptomic and Proteomic Characterization of the Fur Modulon in the Metal-Reducing Bacterium *Shewanella oneidensis*," Xiu-Feng Wan, Nathan C. VerBerkmoes, Lee Ann McCue, Dawn Stanek, Heather Connelly, Loren J. Hauser, Liyou Wu, Xueduan Liu, Tingfen Yan, Adam Leaphart, Robert L. Hettich, Jizhong Zhou, and Dorothea K. Thompson, *J. Bacteriology*, (2004) 186, 8385-8400.
82. "Photochemical Surface Mapping of C14S-Sml1p for Constrained Computational Modeling of Protein Structure," Joshua Sharp, Jun-tao Guo, Tomoaki Uchiki, Ying Xu, Chris Dealwis, and Robert Hettich, *Anal. Biochem.*, 2005,

340, 201-212.

83. "Multipole Storage-Assisted Dissociation (MSAD) for the Characterization of Large Proteins and Protein Mixtures by ESI-FTICR-MS," Chongle Pan and Robert Hettich, Anal. Chem., 2005, 77, 3072-3082.
84. "DBDigger: Reorganized Proteome Database Identification Improves Flexibility and Speed," David Tabb, Chandrasegaran Narasimhan, Michael Strader, and Robert Hettich, Anal. Chem., 2005, 77, 2464-2474.
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.
86. "MASPIC: An intensity based tandem mass spectrometry scoring scheme that improves peptide identification at high confidence," Chandrasegaran (Chandra) Narasimhan, David L. Tabb, Nathan C. VerBerkmoes, Melissa R. Thompson, Robert L. Hettich, and Edward C. Uberbacher, Anal. Chem., (2005) 77, 7581-7593.
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88. "Determination of peptide and protein ion charge states by Fourier transformation of isotope-resolved mass spectra," Tabb DL, Shah MB, Strader MB, Connelly HM, Hettich RL, Hurst GB J. Amer. Soc. Mass Spectrometry (2006) 17 903-915.
89. "Molecular dynamics of the *Shewanella oneidensis* response to chromate stress," Brown SD, Thompson MR, VerBerkmoes NC, Chourey K, Shah M, Zhou JZ, Hettich RL, Thompson DK, Molecular & Cellular Proteomics (2006) 5 1054-1071.
90. "Determination and comparison of the baseline proteomes of the versatile microbe *Rhodopseudomonas palustris* under its major metabolic states," VerBerkmoes NC, Shah MB, Lankford PK, Pelletier DA, Strader MB, Tabb DL, McDonald WH, Barton JW, Hurst GB, Hauser L, Davison BH, Beatty JT, Harwood CS, Tabita FR, Hettich RL, Larimer FW, Journal Of Proteome Research (2006) 5 287-298.
91. "Proteogenomic approaches for the molecular characterization of natural microbial communities," Banfield JF, Verberkmoes NC, Hettich RL, Thelen MP, Omics-A Journal Of Integrative Biology, (2005) 9 301-333.
92. "Characterization of pII family (GlnK1, GlnK2, and GlnB) protein uridylylation in response to nitrogen availability for *Rhodopseudomonas palustris*," Connelly, H. M., Pelletier, D. A., Lu, Tse-Yuan, Lankford, P. K., Hettich, Robert L. Analytical Biochemistry (2006), 357, 93-104.
93. "*ProRata*: A quantitative proteomics program for accurate protein abundance ratio estimation with confidence interval evaluation," Pan, Chongle, Kora, Guruprasad, McDonald, W. Hayes, Tabb, David L., VerBerkmoes, Nathan C., Hurst, Gregory B., Pelletier, Dale A., Samatova, Nagiza F., Hettich, Robert L. Analytical Chemistry (2006) 78, 7121-7131.
94. "Robust estimation of peptide abundance ratios and rigorous scoring of their variability and bias in quantitative shotgun proteomics," Pan, Chongle, Kora, Guruprasad, Tabb, David L., Pelletier, Dale A., McDonald, W. Hayes, Hurst, Gregory B., Hettich, Robert L., Samatova, Nagiza F. Analytical Chemistry (2006) 78, 7110-7120.
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Dissertation Major Advisor - (completed):

- **Dr. Joshua Sharp**, “Development of Hydroxyl Free Radical Chemistry for the Surface Mapping of Proteins,” Ph.D. awarded October 2003. (*academic staff 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 position at UT-El Paso*)
- **Dr. Heather Connolly**, “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 staff position*)
- **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*)

Principal Investigator/Program Director (Last, First, Middle): _____

- **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 ORNL*)
- **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.
- **Dr. Ramsunder (Sarvesh) Iyer**, “Bioinformatic and Experimental Approaches for Deeper Metaproteomic Characterization of Complex Environmental Samples,” Ph.D. awarded August 2017.
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Dissertation Major Advisor (current):

- Ms. Mallory Ladd, graduate student in the ORNL-UTK Bredesen program.
- Mr. Suresh Poudel, graduate student in GST-Ph.D. program
- 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.

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 in the Mass Spectrometry/Laser Spectroscopy Group of the Chemical Sciences Division at Oak Ridge National Laboratory and a joint faculty member in the Microbiology Department at the University of Tennessee. He has over 30 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 220 publications, 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.