Scott R. Kronewitter
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EDUCATION

- **Postdoctoral Research**, Pacific Northwest National Lab, Richland, WA. February 2014
  Focus: Clinical LC-MS Glycomics, Glycoproteomics and Software Development.
  Advisors: Richard D. Smith, Ph.D., Gordon Anderson

- **Ph.D., Analytical Chemistry**, University of California, Davis, CA. February 2010
  Dissertation: Human Serum Glycans as Candidate Biomarkers for Cancer
  Advisor: Carlito B. Lebrilla, Ph.D.

- **M.S., Chemical Engineering**, cum laude, Tufts University, Medford, MA. December 2004
  Thesis: Synthesis and Characterization of Gold Nanoparticles Supported by Polypeptides for Catalytic CO Oxidation. Advisor: Maria Flytzani-Stephanopoulos, Ph.D.

- **B.S., Chemical Engineering**, cum laude, Tufts University, Medford, MA. December 2003

AREAS OF SPECIALIZATION

- Mass spectra data processing, feature detection, and glycan annotation software
  - GlyQ-IQ (C#) and The Glycolyzer V2.0 (C# implementation of the Glycolyzer)
  - LC-MS raw data preprocessing algorithms and feature detection (Thermo/Agilent)
- High Performance Computing
  - Microsoft Windows HPC 2012, Windows Azure Cloud, .Net Framework C#
- Nano LC-MS/MS and MALDI FT-ICR mass spectrometry of N-linked glycans
  - Pack fused silica columns/Gradient optimization of parallel multi-column systems
  - Instrumentation: LC-Orbitrap Velos, LC-SPIN QTOF/Exactive, LC-IMS-QTOF

RESEARCH EXPERIENCE

- **Scientist, Richland, Pacific Northwest National Lab, WA. 2014-Present**
  Microsoft Windows Azure deployment of GlyQ-IQ HPC software.
- **Postdoctoral Research, Pacific Northwest National Lab, Richland, WA. 2010-2014**
  Expanded all aspects of the N-Glycomics analytical pipeline including sample preparation, mass spectrometry and data analysis. Rewriting the Glycolyzer software into C# and the development of the GlyQ-IQ software allowed me to include capabilities to handle nanoESI LC-MS glycan data annotation and quantification for high sensitivity, high specificity and high throughput data analysis. Worked on novel peak detection algorithms to separate MS features from noise. Contributed to PNNL-Omics (C#), DeconTools (C#), and IQ (C#) code bases at PNNL. Wrote the GlyQ-IQ software and deployed it onto HPC clusters at PNNL which utilized 1504 compute cores.

- **Doctoral Research, University of California, Davis, CA. 2004-2010**
  Human serum N-glycan release and purification in preparation for MALDI FT-ICR mass spectrometric analysis. Designed and wrote the Glycolyzer software in IgorPro to automatically pre-process and annotate glycan mass spectra. Additional functionality includes isotope quantification, glycopeptide analysis, and biomarkers hypothesis testing and classification.

- **Masters Research, Tufts University, Medford, MA. 2002-2004**
  Self assembled polypeptide structures used to make gold nanoparticles. Samples were analyzed with HRTEM, time resolved microscopy, time resolved UV-VIS DR, FTIR, XPS, and a catalytic water-gas-shift recycle reactor.

INDUSTRY EXPERIENCE

- **Global Windows Azure Bootcamp, Core Charity Code, HPC Deployment, March 2014**
  http://global.windowsazurebootcamp.com
- **Research Assistant, Hy9 Corporation, Spring 2001-Fall 2001, Summer 2003**
  Non-porous palladium/copper membrane development for hydrogen purification
- **Internship, Millipore Corporation, Summer 2002**
  Protein filter fouling characterization and writing respective analysis software

ACADEMIC ACHIEVEMENTS

- Designed and wrote the Glycolyzer V1.0 glycan mass spectra analysis software
- Extended the PNNL Core software packages to annotate glycomics data
- Built and custom programmed a Gilson ASPEC robotic liquid handler
- Created a theoretical N-linked glycan library for human serum
- Optimized N-linked glycan release and purification sample processing
- Outstanding Performance Award (PNNL, 2011): Robotic Automation
- Outstanding Performance Award (PNNL, 2012): National Security, Breast Cancer Grant

GRANTS

1. **Microsoft Windows Azure Research Pass Grant (2013, Microsoft Research):**
   Allocation of compute time for the high performance computing development of GlyQ-IQ and deployment on the Windows Azure Cloud.
2. **Massively Parallel Molecular Profiling of Breast Cancer (2012, DOD-USAMRAA):**
   Focus on technology applications (for example; proteomics, phosphoproteomics, peptidomics, glycomics) to specific breast cancer phenotype specimens (single time point and longitudinal) for contributing to both a mechanistic understanding of breast cancer as well as for profiling potential candidate biomarkers.

PUBLICATIONS

1. **Scott R. Kronewitter**, Gordon W. Slysz, Ioan Marginean, Clay D. Hagler, Brian L. LaMarche, Rui Zhao, Myanna Y. Harris, Matthew E. Monroe, Christina A. Polyukh, Kevin L. Crowell, Thomas L. Fillmore, Timothy S. Carlson, David G. Camp II, Ronald J. Moore, Samuel H. Payne, Gordon A. Anderson, Richard D. Smith. GlyQ-IQ Part 1: Glycomics Quintavariate-Informed Quantification with High Performance Computing and GlycoGrid 4D Visualization. *Analytical Chemistry*, Submitted, 2014
2. **Scott R. Kronewitter**, Ioan Marginean, Jonathan T. Cox, Rui Zhao, Clay D. Hagler, Anil K. Shukla, Timothy S. Carlson, Joshua N. Adkins, David G. Camp II, Ronald J. Moore, Karin D. Rodland, Richard D. Smith. GlyQ-IQ Part 2: Sensitive Human Serum Glycan Profiling Using Theoretical Retrosynthetic Glycan Libraries, Glycoform Preservation, and Subambient Pressure Electrospray Ionization. *Analytical Chemistry*, In Preparation, 2014
3. John S. Strum, Charles C. Nwosu, Serenus Hua, **Scott R Kronewitter**, Richard R. Seipert, Robert J. Bachelor, Hyun Joo An, Carlito B. Lebrilla. Automated Assignments of N- and O-Site Specific Glycosylation with Extensive Glycan Heterogeneity of Glycoprotein Mixtures. *Analytical Chemistry*, 85, 5666-5675, 2013
4. Brooke L. Deatherage Kaiser, Jie Li, James A. Sanford, Young-Mo Kim, **Scott R. Kronewitter**, Marcus B. Jones, Christine T. Peterson, Scott N. Peterson, Bryan C. Frank, Samuel O. Purvine, Thomas O. Metz, Richard D. Smith, Fred Heffron, and Joshua N. Adkins. A Multi-Omic View of Host-Pathogen-Commensal Interplay in Salmonella-Mediated Intestinal Infection. *PLoS ONE*, 8(6), e67155, 2013
5. Ioan Marginean*, **Scott R. Kronewitter***, Ronald J. Moore, Gordon W. Slysz, Matthew E. Monroe, Gordon Anderson, Keqi Tang, and Richard D. Smith. Improving N-Glycan Coverage using HPLC-MS with Electrospray Ionization at Subambient Pressure. *Analytical Chemistry*. 84(21), 9208-9213, 2012 (*equal contributions towards first author)
6. **Scott R. Kronewitter**, Maria Lorna de Leoz, John S. Strum, Hyun Joo An, Lauren M. Dimapasoc, Andrés Guerrero, Suzanne Miyamoto , Carlito B. Lebrilla, Gary S. Leiserowitz The Glycolyzer: automated glycan annotation software for high performance mass spectrometry and its application to ovarian cancer glycan biomarker discovery. 12(15-16), 2523-2538, *Proteomics*, 2012
7. Tao Liu, Mahmud Hossain, Athena A. Schepmoes, Thomas L. Fillmore, Lori J. Sokoll, **Scott R. Kronewitter**, Grant Izmirlian, Tujin Shi, Wei-Jun Qian, Robin J. Leach, Ian M. Thompson, Daniel W. Chan, Richard D. Smith, Jacob Kagan, Sudhir Srivastava, Karin D. Rodland, David G. Camp II. Analysis of serum total and free PSA using immunoaffinity depletion coupled to SRM: correlation with clinical immunoassay tests. *Journal of Proteomics*, 75(15), 4747-4757, 2012
8. Hyun Joo An, **Scott R. Kronewitter**, Maria Lorna A. de Leoz, Carlito B. Lebrilla. Glycomics and Disease Markers, *Current Opinion in Chemical Biology Journal*, 13(5-6), 601-607, 2009

9. Donald A. Barkauskas, **Scott R. Kronewitter**, Carlito B. Lebrilla, David M. Rocke. Analysis of MALDI FT-ICR Mass Spectrometry Data: A Time Series Approach, *Analytica Chimica Acta*, 648, (2), 207-214, 2009
10. **Scott R. Kronewitter**, Hyun Joo An, Maria Lorna de Leoz, Carlito B. Lebrilla, Suzanne Miyamoto, Gary S. Leiserowitz. The development of retrosynthetic glycan libraries to profile and classify the human serum N-linked glycome, *Proteomics*, 9(11) 2986-2994, 2009
11. Donald A. Barkauskas, Hyun Joo An, **Scott R. Kronewitter**, Maria Lorna de Leoz, Helen K. Chew, Ralph W. de Vere White, Gary S. Leiserowitz, Suzanne Miyamoto, Carlito B. Lebrilla, David M. Rocke. Detecting glycan cancer biomarkers in serum samples using MALDI FT-ICR mass spectrometry data, *Bioinformatics*, 25, 251-257, 2009
12. Riccardo G. LoCascio, Milady R. Niñonuevo, **Scott R. Kronewitter**, Samara L. Freeman, J. Bruce German, Carlito B. Lebrilla, David A. Mills. A versatile and scalable strategy for glycoprofiling bifidobacterial consumption of human milk oligosaccharides, *Microbial Biotechnology*, 2(3), 333-342, 2009
13. Maria Lorna A. de Leoz, Hyun Joo An, **Scott Kronewitter**, Jaehan Kim, Sean Beecroft, Ruth Vinall, Suzanne Miyamoto, Ralph de Vere White, Kit S. Lam, Carlito B. Lebrilla. Glycomic approach for potential biomarkers on prostate cancer: Profiling of N-linked glycans in human sera and pRNS cell lines, *Disease Markers*, 25(4-5), 243-258, 2008

PRESENTATIONS AND CONFERENCES

- **Society for Glycobiology Conference, 2013, St. Petersburg, Florida**
- High-Throughput Human Serum N-Glycan Profiling with GlycoGrid 4D Visualization and Automated Annotation Using GlyQ-IQ Multi-Core Software and High Performance Computing (Poster)
- **American Society of Mass Spectrometry Conference, 2012, Vancouver Canada**
  Global Serum Deglycosylation in High Throughput LC-MS Glycomics: Enhanced Data Clarity via Improved Enzyme Release, Reduction, NanoLC, and IMS-QTOF (Poster)
  Increasing Analyte Ion Charge States via Sub-ambient Pressure Ionization with Nanoelectrospray (Presentation, Ioan Marginean)
- **American Society of Mass Spectrometry Conference, 2011, Denver**
  Global Deglycosylation in High Throughput LC-MS Glycomics: Comparing Microwave, Barocycling, and Ultrasound Effects on PNGase F with Human Serum **(Poster)**
- **American Society of Mass Spectrometry Conference, 2010, Salt Lake City**
  New Strategies for High Pressure-Assisted Digestion in Proteomics (Poster, Kim Hixson)
- **American Society of Mass Spectrometry Conference, 2009, Philadelphia**
  The Development of Methods Towards High Throughput Clinical Glycomics (Presentation)
- **North American FT MS Conference, 2009, Key West**
  High Throughput Software Designed for Cancer Biomarker Discovery in Serum Incorporating Deisotoping, Calibration, and Clinical Testing (Poster and Presentation)

- **Lake Arrowhead Ion Chemistry Conference, 2009, Lake Arrowhead**
  A Theoretical Glycan Library and Applications to Cancer Detection in Serum (Presentation)
- **American Society of Mass Spectrometry Conference, 2008, Denver**
  High Throughput Software Designed for Glycan Biomarker Discovery in Serum Incorporating Deisotoping, Calibration and Spectra Quality Control (Poster)
- **San Diego Glycobiology Symposium, 2008, San Diego**
  Human Serum N-Linked Glycan Mass Profiling: Important Considerations for Spectral Annotation (Poster)
- **American Society of Mass Spectrometry Conference, 2007, Indianapolis**
  An Automated Approach for Assigning Monosaccharide Composition to High-Resolution Mass Spectra of Carbohydrates Using a Combination of Orthogonal Computational Algorithms (Poster)

AMERICAN SOCIETY OF MASS SPECTROMETRY SHORT COURSES

- Ion Mobility Mass Spectrometry, 2011
- High Resolution LC/MS, Philadelphia, 2009
- FTMS Principles and Applications, Denver, 2008

PROFESSIONAL AFFILIATIONS

- American Society of Mass Spectrometry
- American Institute of Chemical Engineers

COLLABORATORS

- Yoshihiro Kawaoka, Ph. D., UW Madison School of Veterinary Medicine
- Minnie Sarwal, MD, MRCP, DCH, Ph.D, The BIOMARC Institute for Personalized Medicine and Theranostics at Sutter Health
- Helen Chew, MD, UC Davis Medical Center
- Gary S. Leiserowitz, MD, UC Davis Medical Center
- David M. Rocke, Ph.D., UC Davis Statistics
- Donald A. Barkauskas, Ph.D., UC Davis Statistics

TEACHING EXPERIENCE

- Mentored Young Women in Science Students: Christina Polyukh, Myanna Harris, 2013
- Mentored Young Women in Science Students: Christina Polyukh, Myanna Harris, 2012
- Mentored UC Davis Early Academic Outreach Program : Kelly McBride, 2007
- Head Teaching Assistant, General Chemistry, UC Davis, Spring 2007
- Teaching Assistant, Analytical Chemistry, UC Davis, Winter 2007
- Teaching Assistant, General Chemistry, UC Davis, Fall 2005, Winter/Spring/Fall 2006

PERSONAL INTERESTS

- Constructed a prototype passively cooled, liquid cooled, personal computer, WA, 2012
- Student at Ultimate Dancesport, Sacramento, CA, 2005-2010
- Tufts University Competitive Ballroom Dance Team, Captain, Medford, MA, 1999-2004
- Executive Board and Ballroom Dance Team Instructor, Medford, MA, 2001-2004
- First Place at the USABDA Intercontinental Dancesport Festival, Daytona Beach, FL, 2001

REFERENCES

Richard D. Smith, Ph.D. dick.smith@pnnl.gov, 509-371-6576
(Chief Scientist Biological Sciences Division, Pan-Omics Mentor, PNNL)
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