

# Daniel Graham Delafield, Ph.D.

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## Employment & Experience

- July 2023 – Present: **Scientist**, Calico Life Sciences
  - Initiated and validated an automated platform for Affinity-Selection Mass-Spectrometry (AS-MS) enabling >24x higher throughput in peptide therapeutic discovery.
  - Applied AS-MS platform to screen >7,000,000 rational design peptide candidates against 8 different targets of interest with 4 yielding high affinity candidates.
  - Implemented an automated pipeline for metabolic stability assays, data collection, and data extraction, providing >\$150,000 cost savings in peptide drug discovery and assessment.
  - Lead efforts to establish and scale internal drug permeability assays, providing a high-throughput platform that enables drug redesign based on molecular properties.
  - Utilized targeted engagement assay technologies (SPP, PISA) to establish drug-protein and library-protein interaction, as well as drug off-target interactions.
  - Employed quantitative proteomics and lectin-based glycopeptide enrichment for identification of protein targets promoting tumor metastasis.
- August 2018 – July 2023: **Research Assistant**, University of Wisconsin-Madison
  - Fabricated and validated PGC-enabled nano separation methodologies that provide up to 40% greater protein, peptide, and glycopeptide identifications.
  - Identified chromatographic conditions most suitable for glycopeptide label-free quantitation, isomeric resolution, or MS-based profiling depth.
  - Utilized DIA-MS to identify 1,245 proteins across six dysregulation patterns correlated with early-, mid-, and late-stage prostate cancer.
  - Coupled machine learning with DIA-MS to quantify >9,300 cerebrospinal fluid proteins and elucidate 1,642 putative neurological disease markers across patient cohorts.
  - Deployed custom web-application solutions for browsing, filtering, and sharing mass spectrometry data.
- June 2021 – August 2021: **Summer Research Intern**, Genentech
  - Developed custom, full-stack desktop applications to automate and streamline immunogenicity assessment of drug candidates, which enabled > 99% reduction in analysis time.
  - Engineered custom user interfaces to enable high-throughput analysis of large tabular datasets, providing a 500-fold increase in data utilization.
  - Constructed analysis pipelines leading to the discovery of constitutive immunogenic signatures that enable reliable quality control in immunopeptidomic workflows.
- 2019 – May 2023: **Ambassador**, Wisconsin Alumni Research Foundation
  - Participated in US patent application, technology disclosure and discussions over viable paths toward intellectual property protection.
  - Identified novel scientific intellectual property from a personal academic network of 300+ graduate students and 50+ principal investigators.
  - Implemented new outreach events, canvas campaigns, and network opportunities aimed toward educating investigators about intellectual property protection, management, and licensing.
  - Augmented the \$3 Billion+ WARF portfolio through the addition of novel gene-edited cell line technologies.

## Education

### DOCTOR OF PHILOSOPHY | MARCH 2023 | UNIVERSITY OF WISCONSIN-MADISON

- Primary Field: Chemistry
- Division: Analytical Chemistry
- GPA: 4.0

### MASTER OF SCIENCE | MAY 2018 | UNIVERSITY OF OKLAHOMA

- Primary Field: Chemistry
- Division: Analytical Chemistry
- GPA: 3.9

## **BACHELOR OF SCIENCE | MAY 2016 | UNIVERSITY OF OKLAHOMA**

- Major: Biochemistry
- Minor: Music
- Honors: Cum Laude

## **Skills**

### **· Proteomics, -omics**

- High-throughput bottom-up, top-down, and middle-down proteomics.
- Label-free and isobaric (Tandem Mass Tag) labeling relative quantitation.
- Affinity-selection mass-spectrometry (AS-MS).
- PTM identification and localization.
  - Glycan, glycopeptide, glycoprotein enrichment, identification, characterization and quantification.
  - Phosphoproteomics.
- Target engagement analysis.
  - Thermal/solvent proteome profiling (TPP/SPP).
  - Proteome integral solubility alteration.
- Small molecule absolute quantification.

### **· Mass Spectrometry**

- Expertise in use, troubleshooting, and maintenance for all major vendors: ThermoFisher, Bruker, Agilent, Waters.
- Data-dependent and data-independent acquisition.
- Parallel reaction monitoring.
- CID, HCD, ETD.

### **· ADME / DMPK**

- Metabolic stability in plasma, serum, gastrointestinal fluids, liver microsomes, cell lysate, cell culture media.
- Drug metabolite identification (MetID) utilizing untargeted mass spectrometry, with an emphasis in canonical and non-canonical peptide drugs.
- Parallel Artificial Membrane Permeability Assay (PAMPA). Uni- and bidirectional.
- Madin Darby Canine Kidney (MDCK) permeability assay. Uni- and bidirectional, MDR1 +/-, with and without p-gp inhibitors.

### **· Liquid-Chromatography, Separations**

- Reversed-phase liquid chromatography (RPLC).
- Porous graphitic carbon (PGC).
- Ion exchange chromatography (IEX).
- Size exclusion chromatography (SEC).
- Capillary electrophoresis – CZE and microfluidic CZE.
- Ion mobility (TIMS, DTIMS, FAIMS).

### **· Computer Science**

- Backend/Data Analysis: Python, R, SQL, Rust
- Frontend: Javascript, HTML, CSS
- General: High throughput analysis, process automation, machine learning, web development.

### **· Professional**

- Written communication.
- Oral communication.
- Project management.
- Mentorship.
- Public speaking.
- Manuscript authorship

## Publications

- **D.G. Delafield**, H.N. Miles, T.N. Liu, W.A. Ricke, L. Li. (2023) "Inclusion of Porous Graphitic Carbon Chromatography Yields Greater Protein Identification, Compartment and Process Coverage, and Enables More Reflective Protein-Level Label-Free Quantitation." *Journal of Proteome Research*. Published online October 10, 2023. 10.1021/acs.jproteome.3c00373
- **D.G. Delafield**, H.N. Miles, W.A. Ricke, L. Li (2022). "Higher Temperature Porous Graphitic Carbon Separations Differentially Impact Distinct Glycopeptide Classes." *Journal for the American Society for Mass Spectrometry*. Published online November 30, 2022. 10.1021/jasms.2c00249
- **D.G. Delafield**, C. Kaminsky, G. Liu, L. Li. (2022) "High-End Ion Mobility Mass Spectrometry: A Current Review of Analytical Capacity in Omics Applications and Structural Investigations." *Trends in Analytical Chemistry*. Published online August 24, 2022. 10.1016/j.trac.2022.116761.
- **D.G. Delafield**, H.N. Miles, Y. Liu, W.A. Ricke, L. Li, (2021). "Complementary Proteome and Glycoproteome Access Revealed Through Comparative Analysis of Reversed Phase and Porous Graphitic Carbon Chromatography." *Analytical Bioanalytical Chemistry*. Invited contribution to the topical paper collection featuring **Promising Early- Career (Bio-)Analytical Researchers**. Published online February 9, 2022. 10.1007/s00216-022-03934-7.
- **D.G. Delafield**<sup>†</sup>, H.N. Miles<sup>†</sup>, L. Li, (2021). "Recent Developments and Applications of Quantitative Proteomics Strategies for High-Throughput Cancer Biomolecular Analyses in Cancer Research. *RSC Chemical Biology*. Published online May 15, 2021. 10.1039/D1CB00039J. († Co-First Authors)
- **D.G. Delafield**, Li, L., (2020) "Recent Advances in Analytical Approaches for Glycan and Glycopeptide Quantitation." *Molecular & Cellular Proteomics*. Published online June 23, 2020. 10.1074/mcp.R120.002095.
- **D.G. Delafield**, H.N. Miles, W.A. Ricke, L. Li. "Proteomic Fingerprinting of Prostate Cancer Progression Through Library-Free DIA-MS Reveals Systematic and Conserved Pathway Dysregulation." (In Submission)
- **D.G. Delafield**<sup>†</sup>, X. Zhong<sup>†</sup>, L. Li. "Sample Agnostic Spectral Libraries Enable Quantitation of >9,300 Cerebrospinal Fluid Proteins Across Neurodegenerative Disease Patient Cohorts." (In Submission) († Co-First Authors)
- **D.G. Delafield**, N. Truettner, H.N. Miles, W.A. Ricke, L. Li, "Capsule Network Retention Time Correction Facilitates Prostatic Tumorigenesis Discovery Through Porous Graphitic Carbon DIA-MS." (In Preparation)
- **D.G. Delafield**, H.N. Miles, W.A. Ricke, L. Li. "Temporal Proteomic Analysis of Progressive Prostate Cancer Model Reveals Concise Therapeutic Targets." (In Preparation)
- **D.G. Delafield**<sup>†</sup>, X. Zhong<sup>†</sup>, L. Li. "Enhanced Proteomic Coverage Enabled through BoxCar DIA and Sample Agnostic Spectral Libraries." (In Preparation) († Co-First Authors)
- Y. Liu, **D.G. Delafield**, L. Li "Comprehensive Mass Spectrometric Characterization of Neuropeptidome in Nervous System of the Atlantic Blue Crab, *Callinectes sapidus*," *Analytical Chemistry*, to be submitted.
- S. Xu, Z. Zhu, T.J. Gu, Z. Wang, **D.G. Delafield**, M.J. Rigby, G. Lu, M. Ma, P. Liu, L. Puglielli, L. Li, "sn-position Resolved Quantification of Aminophospholipids by Isotopic N, N-Dimethyl Leucine Labeling and High-resolution Ion Mobility Mass Spectrometry." *Analytical Chemistry*. Published online December 4, 2024. 10.1021/acs.analchem.4c05107
- S. Xu, Z. Zhu, **D.G. Delafield**, M.J. Rigby, G. Lu, L. Puglielli, L. Li, "Spatially and Temporally Probing Distinctive Glycerophospholipid Alteration In Alzheimer's Disease Mouse Brain Via High-Resolution Ion Mobility-Enabled sn-Position-Resolved Lipidomics." *Nature Communications*. Published online July 24, 2024. doi.org/10.1038/s41467-024-50299-9.
- M. Ma, Q. Yu, **D.G. Delafield**, Y. Cui, Z. Li, W. Wu, X. Shi, A. Gutierrez, P.R. Westmark, M. Xu, C.J. Westmark, L. Li (2023) "On-tissue Spatial Proteomics Integrating MALDI-MS Imaging with Shotgun Proteomics Reveals Soy Consumption-induced Biomarkers in a Fragile X Syndrome Mouse Model." *ACS Chemical Neuroscience*. Published online December 18, 2023. 10.1021/acschemneuro.3c00497.
- Z. Zhu, S. Xu, Z. Wang, **D.G. Delafield**, M.J. Rigby, G. Lu, T. Gu, P. Liu, M. Ma, L. Puglielli, L. Li, (2023) "Chiral Pair Isobaric Labeling Strategy for Multiplexed Absolute Quantitation (CHRISTMAS) Enabled Quantitatively Probing of Enantiomeric Amino Acids Alteration in Alzheimer's Disease Progression," *Analytical Chemistry*. Published online November 30, 2023. 10.1021/acs.analchem.3c03847.

- G. Li, C.K. Jeon, M. Ma, Z. Zheng, Y. Jia, Z. Zheng, **D.G. Delafield**, G. Lu, E. Romanova, J. Sweedler, B. Ruotolo, L. Li, (2023) "Site-specific Chirality-conferred Structural Compaction Differentially Rescues the Cytotoxicity of A $\beta$ 42." *Chemical Science*. Published online May 8, 2023. 10.1039/D3SC00678F
- H. Zhang, **D.G. Delafield**, L. Li. (2023) "Mass spectrometry imaging: the rise of spatially resolved single-cell omics." *Nature Methods*. Published online March 10, 2023. 10.1038/s41592-023-01774-6
- Y Shi, Z. Li, B. Wang, Z. Ye, H. Ye, **D.G. Delafield**, X. Shi, Z. Chen, F. Ma, L. Li (2022) "Enabling Global Analysis of Protein Citrullination and Homocitrullination via Biotin Thiol Tag-Assisted Mass Spectrometry." *Analytical Chemistry*. Published online December 13, 2022. 10.1021/acs.analchem.2c03844.
- N. Wang, N. Wang, S. Yu, H. Zhang, S. Tang, D. Wang, W. Lu, H. Li, **D.G. Delafield**, Y. Kong, X. Wang, C. Shao, L. Lv, G. Wang, R. Tan, N. Wang, H. Hao, H. Ye (2022) "Cyclic Immonium Ion of Lactyllysine Reveals Widespread Lactylation in the Human Proteome," *Nature Methods*. Published online June 28, 2022. 10.1038/s41592-022- 01523-1.
- Z. Li, D. M. Tremmel, F. Ma, Q. Yu, M. Ma, **D.G. Delafield**, Y. Shi, B. Wang, S. A. Mitchell, A. K. Feeney, V. S. Jain, S. D. Sackett, J. S. Odorico, L. Li (2020) "Proteome-wide and Matrisome-specific Alterations during Human Pancreas Development and Maturation," *Nature Communications*. Published online February 15, 2021. 10.1038/s41467- 021-21261-w.
- Ruiz, M., Y. Yang, C. A. Lochbaum, **D. G. Delafield**, J. J. Pignatello, L. Li and J. A. Pedersen (2019). "Peroxymonosulfate Oxidizes Amino Acids in Water without Activation." *Environmental Science and Technology*. 53, 10845-10854.
- Li, G., **D.G. Delafield**, L. Li (2019). "Improved Structural Elucidation of Peptide Isomers and Their Receptors Using Advanced Ion Mobility-Mass Spectrometry." *Trends in Analytical Chemistry*. Published online, June 4, 2019. 10.1016/j.trac.2019.05.048.
- Ma, H., **D. G. Delafield**, Z. Wang, J. You and S. Wu (2017). "Finding Biomass Degrading Enzymes Through an Activity-Related Quantitative Proteomics Platform (ACPP)." *Journal of the American Society for Mass Spectrometry*. 28, 655-663.

## Presentations

- **Delafield, D.G.**; Miles, H.N; Liu, T.N.; Ricke, W.A.; Li, L. "Revealing Systematic Proteomic Remodeling through Library-Free DIA-MS Analysis of a Novel Progressive Prostate Cancer Cell Model" US HUPO 2023 (poster)
- **Delafield, D.G.**; Li, L. "Evaluation of Porous Graphitic Carbon at Elevated Temperatures for Glycopeptide Analyses: Impacts on Signal Suppression, Reduced Identification and Quantitative Inaccuracies" ASMS 2022 (poster).
- **Delafield, D.G.**; Zhong, X.; Yu. Q.; Sauer, C.S.; Zetterberg, H.; Li. L. "Sample Agnostic Spectral Libraries: An Open Framework for Enhanced Data Independent Analysis Profiling Depth" Wisconsin Proteomics Symposium 2022 (**oral**)
- **Delafield, D.G.**; Xia, J.; Li, L. "High Resolution Demultiplexing Ion Mobility: A New Paradigm for Intact Glycopeptide Structural Assignment" ASMS 2021 (poster).
- **Delafield, D.G.**; Cui, Y.; Li, L. "Uncovering Glycoprotein Structural and Compositional Heterogeneity Through Capillary Electrophoresis-Ion Mobility Mass Spectrometry" ACS Fall Meeting 2021 (**oral**).
- **Delafield, D.G.**; Li, L. "Enhancing Glycopeptide Detection, Identification, and Structural Characterization through PGC-Incorporated LC-MS" Pittcon 2021 (**oral**).
- **Delafield, D.G.**; Li, L. "Enhancing Glycopeptide Detection, Identification, and Structural Characterization through PGC-Incorporated LC-IMS" ASMS 2020 (poster).
- **Delafield, D.G.**; Li, G.; Li, L. "Pursuit of Bottom-Up, Middle-Down, and Top-Down Glycoconjugate Analysis Enabled Through Online CE-ESI-IMS" ASMS 2019 (poster).
- **Delafield, D.G.**; Wang, Z.; Baird, M.A.; Shvartsburg, A.; Wu, S. "Characterization Analysis of Glycopeptides Through Arrival Time Correlation using Concurrent RPLC Fraction Monitoring and FAIMS Filtering" ASMS 2018 (poster).
- **Delafield, D.G.**, N-Glycopeptide Feature Identification by Revealing Trends Between Analyte Composition and Compensation Field Through FAIMS-Coupled MS Platform" US HUPO 2018 (**oral**).

- **Delafield, D.G.;** Wang, Z.; Baird, M.A.; Shvartsburg, A.; Smith, K.; Wu, S. “Three-Dimensional Platform for N-Linked Glycopeptide Separation and Analysis” ASMS 2017 (poster).
- **Delafield, D.G.;** Wang, Z.; Woodard, T. Wu, S. “Magnetic Resin Microreactor for Affinity-Capture Top-Down Mass Spectrometry” ASMS 2016 (poster).

## Research Experience

### UNIVERSITY OF WISCONSIN-MADISON, LINGJUN LI LAB

- **Graduate Research/Teaching Assistant**, August 2018 – July 2023
  - Fabricated and validated PGC-enabled nano separation methodologies that provide up to 40% greater protein, peptide, and glycopeptide identifications.
  - Identified chromatographic conditions most suitable for glycopeptide label-free quantitation, isomeric resolution, or MS-based profiling depth.
  - Utilized DIA-MS to identify 1,245 proteins across six dysregulation patterns correlated with early-, mid-, and late-stage prostate cancer.
  - Coupled machine learning with DIA-MS to quantify >9,300 cerebrospinal fluid proteins and elucidate 1,642 putative neurological disease markers across patient cohorts.
  - Deployed custom web-application based solutions for browsing, filtering, and sharing mass spectrometry data.
  - Implementation of informatics pipelines to establish inter- and intrasample quantitative accuracy in data-independent acquisition bottom-up proteomics.
  - Performed custom informatic analysis of MALDI-MSI datasets to normalize multiplexed datasets, extract features of interest, and perform machine learning classification.
  - Development of novel online multiplexed analysis of bottom-up, middle-down, and top-down glycoconjugate species utilizing capillary electrophoresis, porous graphitized carbon liquid chromatography, ion mobility spectrometry, and mass spectrometry.
  - Leveraged custom liquid chromatography, capillary electrophoresis, and ion mobility to identify multiple conformations of active biomolecules.
  - Trained and led small research teams of new graduate students and non-expert scientists in the areas of biomolecular analysis, bioinformatic processing, and project development.
  - Maintained, serviced, and assisted in troubleshooting a variety of high-end mass spectrometers from all major vendors (Thermo, Bruker, Agilent).

### UNIVERSITY OF OKLAHOMA, SI WU LAB

- **Graduate Research/Teaching Assistant**, May 2016 – August 2018
  - Developed a three-dimensional method of glycopeptide purification and characterization allowing universal application, unbiased separation, and rapid recognition using HPLC, concurrent fractionation, Mass Spectrometry, and Differential Ion Mobility (FAIMS). Presented at ASMS, June 2017.
  - Demonstrated correlation between differential ion mobility detection and glycopeptide analytes based on backbone variation, glycan composition, and a combination thereof.
  - Analyzed post translationally modified glycoproteins of control and SLE patient serum immunoglobulin searching for correlations to immune response and glycan features based on our previous glycopeptide purification platform.
- **Honors Research Assistant**, January 2016 – May 2016
  - Conceptualized, designed, and constructed an online affinity capture technique for immunoprecipitation application involving intensive immunoglobulin purification, original apparatus design, and top-down mass spectrometry. ASMS, June 2016.
- **Undergraduate Research Assistant**, August 2015 – January 2016
  - Determined activity of novel biomass degrading enzymes from Great Lakes fungal samples through culturing, secretome extraction, enzymatic assays, concentration determination, electrophoresis, liquid chromatography and mass spectrometry. Published in JASMS, April 2017 (Online January 2017).

## Funding

- DiLeu-Enabled Mutiplexed Quantitation for Biomarker Discovery and Validation in Alzheimer’s Disease (Renewal)

- Role: Contributing Author
- Funding Amount: \$2,835,460
- Creating a Region-Specific Biomolecular Atlas of the Brain in Alzheimer's Disease (1R01AG078794-01, September 2022)
- Role: Contributing Author
- Funding Amount: \$3,780,730
- Acquisition of a Dual-Source, High-Performance, Ion Mobility, Quadrupole Time-of-Flight Mass Spectrometry System for Biomedical Research at UW-Madison (1S10OD028473-01A1, May 2021)
- Role: Primary Author
- Funding Amount: \$1,275,704

## Awards and Honors

- **2023:** Gary Parr Memorial Award for Outstanding Bioanalytical Graduate Research
- **2022:** Luminex Summer Fellowship
- **2022:** Chemistry Department Travel Award
- **2022:** Department of Chemistry Harold Hay Fellowship
- **2019:** Student Research Travel Grant
- **2018:** Honored Instructor Award
- **2018:** ASMS Travel Grant
- **2017:** Head Teaching Assistant
- **2017:** Certificate of Distinction in Teaching
- **2017:** College of Arts & Sciences Travel Grant
- **2016:** Scott Laing Outstanding Undergraduate Research Award
- **2016:** Honors Research Assistant
- **2016:** Outstanding Senior Man Award
- **2016:** J. Lee Burke Outstanding Student Achievement Award

## Mentorship, Teaching & Community Involvement

- **Contractor Co-advisor**, August 2023-Present
  - Designed experiments related to peptide affinity selection assays, automated assay validation, quantitative target engagement analyses and extracellular matrix protein identification.
  - Designed and guided experiments for education on a teach-together-learn model.
  - Advised strategies for personal development, project management, and data presentation.
- **Graduate Mentor**, January 2023-May 2023
  - Conceived project for informatics-driven retention time calibration for discovery-based DIA-MS data collection.
  - Taught fundamental sample preparation, mass spectrometry, liquid chromatography concepts.
  - Taught data-science-like concepts such as high-throughput data ingestion, cleaning, parsing, and analysis.
- **Graduate Mentor**, January 2022-May 2022
  - Designed research project centering on the analysis of lipochitooligosaccharides (LCOs) from fungal extracts
  - Taught fundamental sample preparation, mass spectrometry, liquid chromatography concepts
  - Instructed and guided molecule search space database creation and data querying
- **Teaching Assistant**, August 2018-May 2019
  - Formulated and delivered bi-weekly lesson plans based on outlined course objectives.
  - Assisted in exam writing and proofing.
  - Aided student groups in the development of unique experiment design and result presentation.
- **Head Teaching Assistant**, August 2017-May 2018
  - Coordinated teaching schedules, materials, and lesson plans for 57 Teaching Assistants across 71 classes.
  - Served as primary contact between professors of record and 2,000+ undergraduate students.
  - Led teaching assistants through development of weekly instruction, grading expectations, and lesson preparation.
  - Reviewed and rewrote exam material based on learning objectives.
- **Teaching Assistant**, August 2016-May 2017

- Designed interactive lessons based on course learning objectives.
- Promoted individual and group demonstration of knowledge.
- Created, submitted, explained, and graded weekly assignments.
- **Norman North High School, 2015-2017**
  - Formulated and implemented lesson plans for groups small and large.
  - Assisted team members in goal-based teaching strategies.
  - Adapted learning concepts to promote growth and retention.

## **Professional Affiliations**

- **American Society for Mass Spectrometry (ASMS)**
- **United States Human Proteome Organization (U.S. HUPO)**