

William E Fondrie, PhD

Talus Bioscience
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Updated August 19, 2024.

Education

- 2013–18 **PhD in Molecular Medicine**
University of Maryland, Baltimore
Advisors: David Goodlett, PhD and Dudley Strickland, PhD
- 2009–13 **BS in Chemistry**
University of North Carolina at Chapel Hill

Employment and Professional Appointments

- 2024– **Head of Data Science and Engineering**, Talus Bioscience
- 2022–24 **Manager, Computational Biology**, Talus Bioscience
- 2021–22 **Senior Data Scientist**, Talus Bioscience
- 2019–21 **University of Washington Data Science Postdoctoral Fellow**
UW eScience Institute
- 2018–21 **Postdoctoral Fellow**, University of Washington
Advisor: William Noble, PhD
- 2013–18 **Graduate Research Assistant**, University of Maryland, Baltimore
Advisors: David Goodlett, PhD and Dudley Strickland, PhD
- 2012–13 **Undergraduate Research Assistant**, University of North Carolina at Chapel Hill
Advisor: John Papanikolas, PhD

Awards and Honors

- 2021 **Rising Stars in Proteomics and Metabolomics: 40 under 40**,
Journal of Proteome Research
- 2020 **Emerging Talent: Academia**, American Society for Mass Spectrometry
- 2019–21 **Ruth L Kirschstein Institutional National Research Service Award**
NIH T32HG000035, Postdoctoral Trainee
- 2017 **Travel Fellowship to the May Institute on Computation and Statistics for Mass Spectrometry and Proteomics**
- 2017–18 **Ruth L Kirschstein Individual National Research Service Award**
NIH F31CA213815, PI
- 2016–17 **Ruth L Kirschstein Institutional National Research Service Award**
NIH T32HL007698, Predoctoral Trainee
- 2012 **Markham Summer Undergraduate Research Award**
- 2009 **Central Carolina's chapter of Phi Beta Kappa Scholarship**

Preprints

(* indicates equal contributions)

- (2) Vollger MR, Swanson EG, Neph SJ, Ranchalis J, Munson KM, Ho C, Sedeño-Cortés AE, **Fondrie WE**, Bohaczuk SC, Mao Y, Parmalee NL, Mallory BJ, Harvey WT, Kwon Y, Garcia GH, Hoekzema K, Meyer JG, Cicek M, Eichler EE, Noble WS, Witten DM, Bennett JT, Ray JP, Stergachis AB. (2024) A Haplotype-Resolved View of Human Gene Regulation. *bioRxiv*, 2024.06.14.599122. <https://doi.org/10.1101/2024.06.14.599122>
- (1) Bittremieux W, Ananth V, **Fondrie WE**, Melendez C, Pominova M, Sanders J, Wen B, Yilmaz M, Noble WS. (2024) Deep Learning Methods for de Novo Peptide Sequencing. *ChemRxiv*, <https://doi.org/10.26434/chemrxiv-2024-l6wnt>

Peer-Reviewed Publications

(* indicates equal contributions)

- (23) Yilmaz M, **Fondrie WE**, Bittremieux W, Melendez CF, Nelson R, Ananth V, Oh S, Noble WS. (2024) Sequence-to-Sequence Translation from Mass Spectra to Peptides with a Transformer Model. *Nature Communications*, 15(1),6427. <https://doi.org/10.1038/s41467-024-49731-x>
- (22) Lin A, See D, **Fondrie WE**, Keich U, Noble WS. (2024) Target-Decoy False Discovery Rate Estimation Using Crema. *Proteomics*, 24(8),e2300084. <https://doi.org/10.1002/pmic.202300084>
- (21) Harris L, **Fondrie WE**, Oh S, Noble WS. (2023) Evaluating Proteomics Imputation Methods with Improved Criteria. *Journal of Proteome Research*, 22(11),3427–3438. <https://doi.org/10.1021/acs.jproteome.3c00205>
- (20) Allen C, Meinl R, Paez JS, Searle BC, Just S, Pino LK, **Fondrie WE**. (2023) Nf-Encyclopedia: A Cloud-Ready Pipeline for Chromatogram Library Data-Independent Acquisition Proteomics Workflows. *Journal of Proteome Research*, <https://doi.org/10.1021/acs.jproteome.2c00613>
- (19) Arab I, **Fondrie WE**, Laukens K, Bittremieux W. (2023) Semisupervised Machine Learning for Sensitive Open Modification Spectral Library Searching. *Journal of Proteome Research*, 22(2),585–593. <https://doi.org/10.1021/acs.jproteome.2c00616>
- (18) Kertesz-Farkas A, Nii Adoquaye Acquaye FL, Bhimani K, Eng JK, **Fondrie WE**, Grant C, Hoopmann MR, Lin A, Lu YY, Moritz RL, MacCoss MJ, Noble WS. (2023) The Crux Toolkit for Analysis of Bottom-Up Tandem Mass Spectrometry Proteomics Data. *Journal of Proteome Research*, 22(2),561–569. <https://doi.org/10.1021/acs.jproteome.2c00615>
- (17) Heil LR, **Fondrie WE**, McGann CD, Federation AJ, Noble WS, MacCoss MJ, Keich U. (2022) Building Spectral Libraries from Narrow-Window Data-Independent Acquisition Mass Spectrometry Data. *Journal of Proteome Research*, 21(6),1382–1391. <https://doi.org/10.1021/acs.jproteome.1c00895>

- (16) Phipps WS, Smith KD, Yang H, Henderson CM, Pflaum H, Lerch ML, **Fondrie WE**, Emrick MA, Wu CC, MacCoss MJ, Noble WS, Hoofnagle AN. (2022) Tandem Mass Spectrometry-Based Amyloid Typing Using Manual Microdissection and Open-Source Data Processing. *American Journal of Clinical Pathology*, 157(5),748–757. <https://doi.org/10.1093/ajcp/aqab185>
- (15) Yilmaz M, **Fondrie W**, Bittremieux W, Oh S, Noble WS. (2022) De Novo Mass Spectrometry Peptide Sequencing with a Transformer Model. *International Conference on Machine Learning*, 25514–25522.
- (14) **Fondrie WE**, Bittremieux W, Noble WS. (2021) Ppx: Programmatic Access to Proteomics Data Repositories. *Journal of Proteome Research*, 20(9),4621–4624. <https://doi.org/10.1021/acs.jproteome.1c00454>
- (13) Mudge MC, Nunn BL, Firth E, Ewert M, Hales K, **Fondrie WE**, Noble WS, Toner J, Light B, Junge KA. (2021) Subzero, Saline Incubations of Colwellia Psychrerythraea Reveal Strategies and Biomarkers for Sustained Life in Extreme Icy Environments. *Environmental Microbiology*, 23(7),3840–3866. <https://doi.org/10.1111/1462-2920.15485>
- (12) **Fondrie WE**, Noble WS. (2021) Mokapot: Fast and Flexible Semisupervised Learning for Peptide Detection. *Journal of Proteome Research*, 20(4),1966–1971. <https://doi.org/10.1021/acs.jproteome.0c01010>
- (11) **Fondrie WE**, Noble WS. (2020) Machine Learning Strategy That Leverages Large Data Sets to Boost Statistical Power in Small-Scale Experiments. *Journal of Proteome Research*, 19(3),1267–1274. <https://doi.org/10.1021/acs.jproteome.9b00780>
- (10) Liang T, Leung LM, Opene B, **Fondrie WE**, Lee YI, Chandler CE, Yoon SH, Doi Y, Ernst RK, Goodlett DR. (2019) Rapid Microbial Identification and Antibiotic Resistance Detection by Mass Spectrometric Analysis of Membrane Lipids. *Analytical Chemistry*, 91(2),1286–1294. <https://doi.org/10.1021/acs.analchem.8bo2611>
- (9) Au DT, Ying Z, Hernández-Ochoa EO, **Fondrie WE**, Hampton B, Migliorini M, Galisteo R, Schneider MF, Daugherty A, Rateri DL, Strickland DK, Muratoglu SC. (2018) LRP1 (Low-Density Lipoprotein Receptor-Related Protein 1) Regulates Smooth Muscle Contractility by Modulating Ca²⁺ Signaling and Expression of Cytoskeleton-Related Proteins. *Arteriosclerosis, Thrombosis, and Vascular Biology*, 38(11),2651–2664. <https://doi.org/10.1161/ATVBAHA.118.311197>
- (8) **Fondrie WE**, Liang T, Oyler BL, Leung LM, Ernst RK, Strickland DK, Goodlett DR. (2018) Pathogen Identification Direct From Polymicrobial Specimens Using Membrane Glycolipids. *Scientific Reports*, 8(1),15857. <https://doi.org/10.1038/s41598-018-33681-8>
- (7) Liang T, Schneider T, Yoon SH, Oyler BL, Leung LM, **Fondrie WE**, Yen G, Huang Y, Ernst RK, Nilsson E, Goodlett DR. (2018) Optimized Surface Acoustic Wave Nebulization Facilitates Bacterial Phenotyping. *International Journal of Mass Spectrometry*, 42765–72. <https://doi.org/10.1016/j.ijms.2017.09.007>
- (6) Au DT, Arai AL, **Fondrie WE**, Muratoglu SC, Strickland DK. (2018) Role of the LDL Receptor-Related Protein 1 in Regulating Protease Activity and Signaling Pathways in the Vasculature. *Current Drug Targets*, 19(11),1276–1288. <https://doi.org/10.2174/1389450119666180511162048>

- (5) Khan MM, Tran BQ, Jang Y, Park S, **Fondrie WE**, Chowdhury K, Yoon SH, Goodlett DR, Chae S, Chae H, Seo S, Goo YA. (2017) Assessment of the Therapeutic Potential of Persimmon Leaf Extract on Prediabetic Subjects. *Molecules and Cells*, 40(7),466–475. <https://doi.org/10.14348/molcells.2017.2298>
- (4) Leung LM, **Fondrie WE**, Doi Y, Johnson JK, Strickland DK, Ernst RK, Goodlett DR. (2017) Identification of the ESKAPE Pathogens by Mass Spectrometric Analysis of Microbial Membrane Glycolipids. *Scientific Reports*, 7(1),6403. <https://doi.org/10.1038/s41598-017-04793-4>
- (3) Clark DJ, **Fondrie WE**, Yang A, Mao L. (2016) Triple SILAC Quantitative Proteomic Analysis Reveals Differential Abundance of Cell Signaling Proteins between Normal and Lung Cancer-Derived Exosomes. *Journal of Proteomics*, 133161–169. <https://doi.org/10.1016/j.jprot.2015.12.023>
- (2) Clark DJ*, **Fondrie WE***, Liao Z, Hanson PI, Fulton A, Mao L, Yang AJ. (2015) Redefining the Breast Cancer Exosome Proteome by Tandem Mass Tag Quantitative Proteomics and Multivariate Cluster Analysis. *Analytical Chemistry*, 87(20),10462–10469. <https://doi.org/10.1021/acs.analchem.5b02586>
- (1) Ma D, Bettis SE, Hanson K, Minakova M, Alibabaei L, **Fondrie W**, Ryan DM, Papoian GA, Meyer TJ, Waters ML, Papanikolas JM. (2013) Interfacial Energy Conversion in Ru(II) Polypyridyl-Derivatized Oligoproline Assemblies on TiO₂. *Journal of the American Chemical Society*, 135(14),5250–5253. <https://doi.org/10.1021/ja312143h>

Dissertation

- (1) **Fondrie WE**. (2018) Biological Insight from Mass Spectrometry through Novel Computational Approaches.

Patents

- (2) Canzani D, **Fondrie WE**, Pino LK, Federation A. (2023) Methods for identifying reactive functional cysteines in nuclear proteins. WO2023225568A1.
- (1) Goodlett DR, Ernst RK, Liang T, **Fondrie WE**, Nilsson E. (2018) Methods for Lipid Extraction and Identification of Microbes Using Same Via Mass Spectrometry. US Patent Application 2017066342. Filed 12/14/2017. *Patent Pending*.

Grants

- (4) **Deep learning methods to accelerate discovery of drugs targeting gene regulatory proteins.**
Funder: NIGMS 1R43GM146472-01A1
Amount: \$398,441
Period: 2023–2024
Role: PI

- (3) **Activity-based regulome profiling for the discovery of covalent transcription factor inhibitors.**
Funder: NCATS 1R44TR004349-O1
Amount: \$307,465
Period: 2023
Role: Co-I
- (2) **Therapeutic disruption of the Rhabdomyosarcoma transcriptional core regulatory circuit.**
Funder: Andy Hill CARE Fund
Amount: \$1,995,337
Period: 2023–2025
Role: Co-I
- (1) **Illuminating the "dark" kinases - effects on proteome translocation and chromatin binding.**
Funder: NCATS 1R43TR004221-O1
Amount: \$333,867
Period: 2022–2023
Role: Co-I

Scientific Software Contributions

- (16) **depthcharge.** A deep learning toolkit for proteomics data.
Homepage: <https://wfondrie.github.io/depthcharge>
Roles: creator and maintainer
- (15) **Casanovo.** *De novo* peptide sequencing using deep learning.
Homepage: <https://casanovo.readthedocs.io>
Roles: creator and maintainer
- (14) **nf-encyclopedia.** A pipeline for analyzing DIA proteomics data with chromatogram libraries.
Homepage: <https://talusbio.github.io/nf-encyclopedia>
Roles: creator and maintainer
- (13) **mokapot.** A Python package that enables the fast and flexible application of semi-supervised learning to detect peptides in proteomics experiments.
Homepage: <https://github.com/wfondrie/mokapot>
Roles: creator and maintainer
- (12) **ppx.** A Python package for programmatic access to proteomics data repositories.
Homepage: <https://github.com/wfondrie/ppx>
Roles: creator and maintainer
- (11) **quantms.** A NextFlow pipeline for quantitative proteomics.
Homepage: <https://quantms.org/home>
Roles: contributor
- (10) **Sage.** An ultrafast open-modification search engine for proteomics.
Homepage: <https://sage-docs.vercel.app/>
Roles: contributor

- (9) **Comet**. A proteomics search engine.
Homepage: <https://uwpr.github.io/Comet/>
Roles: contributor
- (8) **Crux**. A mass spectrometry toolkit for proteomics data.
Homepage: <http://crux.ms>
Roles: contributor
- (7) **Percolator**. Semi-supervised learning for peptide identification from shotgun proteomics datasets.
Homepage: <http://percolator.ms>
Roles: contributor
- (6) **dask-ml**. A library for distributed and parallel machine learning using dask.
Homepage: <https://ml.dask.org>
Roles: contributor
- (5) **Kojak**. A search engine for cross-linking proteomics.
Homepage: <http://www.kojak-ms.org>
Roles: contributor
- (4) **MSToolkit**. A library for interacting with proteomics data formats.
Homepage: <https://github.com/mhoopmann/mstoolkit>
Roles: contributor
- (3) **ANN-SoLo**. A spectral library search engine for fast and accurate open modification searching.
Homepage: <https://github.com/bittremieux/ANN-SoLo>
Roles: contributor
- (2) **spectrum_utils**. A Python package for efficient MS/MS spectrum processing and visualization.
Homepage: https://github.com/bittremieux/spectrum_utils
Roles: contributor.
- (1) **xComb**. A cross-linked peptide database approach to protein-protein interaction analysis.
Homepage: <https://github.com/GoodlettLab/xComb>
Roles: maintainer and contributor

Invited Talks

- (1) **Fondrie WE**. (2023) The final frontier: These are the voyages through a latent space shared by mass spectra and peptides. *38th Asilomar Conference on Mass Spectrometry*, Pacific Grove, CA

Talks

- (8) Allen C, Paez JS, Gutierrez AI, Robbins JE, Canzani D, Pino LK, Federation AJ, **Fondrie WE**. (2024) The Screen's Gambit: Functional Chemoproteomics Accelerated by Compressed

Sensing and Generative Models. *72nd American Society for Mass Spectrometry Annual Conference on Mass Spectrometry and Allied Topics*, Anaheim, CA

- (7) **Fondrie WE**, Broderick EF, Meinel R, Schumacker NC, Canzani D, Federation AJ, Pino LK. (2022) The Need for Speed: Compressed Sensing With Generative Models Enables Ultra High-Throughput DIA Mass Spectrometry. *70th American Society for Mass Spectrometry Annual Conference on Mass Spectrometry and Allied Topics*, Minneapolis, MN
- (6) **Fondrie WE**, Noble WS, Romero E. (2021) Learning Compact Representations of High-Resolution Tandem Mass Spectra Without Supervision. *69th American Society for Mass Spectrometry Annual Conference on Mass Spectrometry and Allied Topics*, Philadelphia, PA
- (5) **Fondrie WE**, Noble WS, Romero E. (2021) Learning Compact Representations of High-Resolution Tandem Mass Spectra Without Supervision. *Intelligent Systems for Molecular Biology*, Online
- (4) **Fondrie WE**. (2020) Deep Learning to Enable Proteomics at Scale. *American Society for Mass Spectrometry Emergin Talent: Academia webinar series*, Online
- (3) **Fondrie WE**. (2020) Learning from Mass Spectra. *Genome Sciences Seminar*, University of Washington Department of Genome Sciences, Seattle, WA
- (2) **Fondrie WE**, Leung LM, Strickland DK, Ernst RK, Goodlett DR. (2017) Detecting antibiotic resistance by MALDI-TOF analysis of bacterial membrane glycolipids.. *65th American Society for Mass Spectrometry Annual Conference on Mass Spectrometry and Allied Topics*, Indianapolis, IN
- (1) **Fondrie WE**, Muratoglu SC, Hampton B, Migliorini M, Galisteo R, Strickland DK. (2016) LRP1 modulates TGF-beta signaling in the descending thoracic aorta. *Molecular Medicine Research Retreat*, Baltimore, MD

Teaching

Training

2020 The Carpentries Instructor Training
<https://carpentries.org/>

Experience

2022– Machine Learning for Mass Spectrometry Data Analysis, ASMS Annual Conference 2-day short course.

2021 UW Fall Quarter Software Carpentry Workshop Instructor
<https://uwescience.github.io/2021-10-11-uw-online/>

2021 UW Spring Quarter Software Carpentry Workshop Instructor
<https://uwescience.github.io/2021-05-10-uw-online/>

2021 Lecture for the “Statistics for Proteomics” video series
Course website: <https://slavovlab.net/stats>
Lecture: <https://youtu.be/up7B10eedk>

2021 UW Winter Quarter Software Carpentry Workshop Instructor
<https://uwescience.github.io/2021-01-11-uw-online/>

Professional Service

Editorial Boards

2021–23 *Journal of Proteome Research*. Editorial Advisory Board.

Conference Organization

2024 Intelligent Systems for Molecular Biology CompMS COSI. *Program Committee Member*.

2021 Intelligent Systems for Molecular Biology CompMS COSI. *Program Committee Member*.

2020 Workshop on High Performance Computing, Big Data Analytics and Integration for Multi-Omics Biomedical Data (HPC-BOD 2020). *Program Committee Member*.

Professional Memberships

2021– American Chemical Society (ACS)

2021– Human Proteome Organization (HUPO)

2020– United States Human Proteome Organization (US HUPO)

2013– American Society for Mass Spectrometry (ASMS)

Other Service

2023– Bits in Bio City Captain, Seattle Chapter

2019–21 UW Genome Sciences Art Committee

2018–21 Postdoctoral representative in UW Genome Sciences

2015–17 UMB Molecular Medicine Event Planning Committee

2017 UMB Cancer Biology Research Retreat Organizing Committee

2016 UMB Grollman Lecture Organizing Committee

Scientific Blog Posts

- (5) **Fondrie WE.** (2024) Tips for Collaborative Writing with LaTeX and GitHub.
<https://willfondrie.com/2024/02/10-tips-for-collaborative-writing-with-latex-and-github/>
- (4) **Fondrie WE.** (2022) How to Use R Packages in Python.
<https://willfondrie.com/2022/01/how-to-use-r-packages-in-python/>
- (3) **Fondrie WE.** (2022) Why I Joined a Biotech Startup.
<https://willfondrie.com/2021/09/why-i-joined-a-biotech-startup/>
- (2) **Fondrie WE.** (2019) Using Static Models in Percolator.
<https://willfondrie.com/2019/11/using-static-models-in-percolator/>
- (1) **Fondrie WE.** (2019) An Intuitive Look at the xcorr Score Function in Proteomics.
<https://willfondrie.com/2019/02/an-intuitive-look-at-the-xcorr-score-function-in-proteomics/>