William E Fondrie, PhD

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Updated O	ctober 15, 2023.
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
Employme	ent and Professional Appointments
2022-	Manager, Computational Biology, Talus Bioscience
2021-22	Senior Data Scientist, Talus Bioscience
2019-21	University of Washington Data Science Postdoctoral Fellow

2019-21	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, <i>Journal of Proteome Research</i>
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)

(3) Lin A, See D, **Fondrie WE**, Keich U, Noble WS. (2023) Target-Decoy False Discovery Rate Estimation Using Crema. *bioRxiv*, https://doi.org/10.1101/2023.06.18.545038

- (2) Harris L, **Fondrie WE**, Oh S, Noble WS. (2023) Evaluating Proteomics Imputation Methods with Improved Criteria. *bioRxiv*, https://doi.org/10.1101/2023.04.07.535980
- (1) Yilmaz M*, **Fondrie WE***, Bittremieux W, Nelson R, Ananth V, Oh S, Noble WS. (2023) Sequence-to-Sequence Translation from Mass Spectra to Peptides with a Transformer Model. *bioRxiv*, https://doi.org/10.1101/2023.01.03.522621

Peer-Reviewed Publications	

(* indicates equal contributions)

- (19) 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.2co0613
- (18) 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
- (17) 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
- (16) 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
- (15) 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/aicp/agab185
- (14) 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.
- (13) **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

(12) 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

- (11) **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.oco1010
- (10) **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
- (9) 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
- (8) 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
- (7) **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
- (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

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

Patents

(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*.

Scientific Software Contributions

(15) **depthcharge**. A deep learning toolkit for proteomics data.

Homepage: https://wfondrie.github.io/depthcharge

Roles: creator and maintainer

(14) **Casanovo**. De novo peptide sequencing using deep learning.

Homepage: https://casanovo.readthedocs.io

Roles: creator and maintainer

(13) **nf-encyclopedia**. A pipeline for analyzing DIA proteomics data with chromatogram libraries.

Homepage: https://talusbio.github.io/nf-encyclopedia

Roles: creator and maintainer

(12) **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

(11) **ppx**. A Python package for programmatic access to proteomics data repositories.

Homepage: https://github.com/wfondrie/ppx

Roles: creator and maintainer

(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

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(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

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(7) **Fondrie WE**, Broderick EF, Meinl 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/up7Bl0eeedk
2021	UW Winter Quarter Software Carpentry Workshop Instructor https://uwescience.github.io/2021-01-11-uw-online/

Editorial Boards

Professional Service

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

Conference Organization

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

- (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/