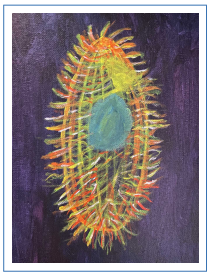
Caitlyn McCafferty

Curriculum Vitae

Biozentrum
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Google Scholar



Education

2017–2022 **PhD, Cell & Molecular Biology**, *University of Texas*, Austin.
Protein-protein interactions, Protein structure, Integrative modeling, Cryo-electron microscopy, Ciliary protein complexes

2015–2017 **Foundation for Advanced Education in the Sciences**, *National Institutes of Health*, Bethesda, MD.
Introduction to Python, Research Tools for Studying Disease, Molecular Modeling and Molecular Dynamics

January,2015 **School of Public Policy**, *University of Maryland*, Indonesia.
Environmental Policy and Sustainability

2011–2015 **Bachelor of Science, Chemistry**, *University of Maryland*, College Park.

Publications

Journal Articles (*indicates corresponding authorship)

2025 **Caitlyn L McCafferty***, Hugo van den Hoek, Marine Brunet, Garrison Buss, et al. **The molecular architecture of the ciliary base in mammalian multiciliated cells**. *Biorxiv*, pages 2025–09. Cold Spring Harbor Laboratory, 2025.

2025 **Caitlyn L McCafferty***, Ophelia Papoulas, Chanjae Lee, Khanh Huy Bui, David W Taylor, Edward M Marcotte, and John B Wallingford. **An amino acid-resolution interactome for motile cilia identifies the structure and function of ciliopathy protein complexes**. *Developmental Cell*, volume 60, pages 965–978. Elsevier, 2025.

2025 **Caitlyn L McCafferty***, Gabriel Hoogerbrugge, Ophelia Papoulas, Evan Schwartz, Simon Ritchey, David W Taylor, Axel Brilot, and Edward M Marcotte. **The CAGE complex: a hollow, megadalton, protein assembly in prokaryotic and eukaryotic microbes**. *Biorxiv*, pages 2025–09. Cold Spring Harbor Laboratory, 2025.

2025 Eloïse Bertiaux, Vincent Louvel, **Caitlyn L McCafferty** McCafferty, Hugo van den Hoek, Umut Batman, et al. **The Luminal Ring Protein C2CD3 Acts as a Radial In-to-Out Organizer of the Distal Centriole and Appendages**. *Biorxiv*, pages 2025–06. Cold Spring Harbor Laboratory, 2025.

2024 **Caitlyn L McCafferty***, Sven Klumpe, Rommie E Amaro, Wanda Kukulski, Lucy Collinson, and Benjamin D Engel. **Integrating cellular electron microscopy with multimodal data to explore biology across space and time**. *Cell*, volume 187, pages 563–584. Elsevier, 2024.

2024 Evan A Schwartz, Jack PK Bravo, Mohd Ahsan, Luis A Macias, **Caitlyn L McCafferty**, Tyler L Dangerfield, Jada N Walker, Jennifer S Brodbelt, Giulia Palermo, Peter C Fineran, et al. **RNA targeting and cleavage by the type III-Dv CRISPR effector complex**. *Nature communications*, volume 15, page 3324. Nature Publishing Group UK London, 2024.

2024 Ron Kelley, Sagar Khavnekar, Ricardo Righetto, ... **Caitlyn L McCafferty**, et al. **Towards community-driven visual proteomics with large-scale cryo-electron tomography of Chlamydomonas reinhardtii**. *bioRxiv*, pages 2024–12. Cold Spring Harbor Laboratory, 2024.

2023 **Caitlyn L McCafferty***, Erin L Pennington, Ophelia Papoulas, David W Taylor, and Edward M Marcotte. **Does AlphaFold2 model proteins' intracellular conformations? An experimental test using cross-linking mass spectrometry of endogenous ciliary proteins**. *Communications Biology*, volume 6, page 421. Nature Publishing Group UK London, 2023.

2023 Shintaroh Kubo, Corbin S Black, Ewa Joachimiak, Shun Kai Yang, Thibault Legal, Katya Peri, Ahmad Abdelzaher Zaki Khalifa, Avrin Ghanaeian, **Caitlyn L McCafferty**, Melissa Valente-Paterno, et al. **Native doublet microtubules from Tetrahymena thermophila reveal the importance of outer junction proteins**. *Nature Communications*, volume 14, page 2168. Nature Publishing Group UK London, 2023.

2023 Avrin Ghanaeian, Sumita Majhi, **Caitlyn L McCafferty**, Babak Nami, Corbin S Black, Shun Kai Yang, Thibault Legal, Ophelia Papoulas, Martyna Janowska, Melissa Valente-Paterno, et al. **Integrated modeling of the Nexin-dynein regulatory complex reveals its regulatory mechanism**. *Nature Communications*, volume 14, page 5741. Nature Publishing Group UK London, 2023.

2022 **Caitlyn L McCafferty***, Ophelia Papoulas, Mareike A Jordan, Gabriel Hoogerbrugge, Candice Nichols, Gaia Pigino, David W Taylor, John B Wallingford, and Edward M Marcotte. **Integrative modeling reveals the molecular architecture of the intraflagellar transport A (IFT-A) complex**. *Elife*, volume 11, page e81977. eLife Sciences Publications Limited, 2022.

2022 Wisath Sae-Lee, **Caitlyn L McCafferty**, Eric J Verbeke, Pierre C Havugimana, Ophelia Papoulas, Claire D McWhite, John R Houser, Kim Vanuytsel, George J Murphy, Kevin Drew, et al. **The protein organization of a red blood cell**. *Cell Reports*, volume 40, page 111103. Elsevier, 2022.

2021 **Caitlyn L McCafferty***, David W Taylor, and Edward M Marcotte. **Improving integrative 3D modeling into low-to medium-resolution electron microscopy structures with evolutionary couplings**. *Protein Science*, volume 30, pages 1006–1021. John Wiley & Sons, Inc. Hoboken, USA, 2021.

2021 **Caitlyn L McCafferty***, Edward M Marcotte, and David W Taylor. **Simplified geometric representations of protein structures identify complementary interaction interfaces**. *Proteins: Structure, Function, and Bioinformatics*, volume 89, pages 348–360. John Wiley & Sons, Inc. Hoboken, USA, 2021.

2020 **Caitlyn L McCafferty**, Eric J Verbeke, Edward M Marcotte, and David W Taylor. **Structural Biology in the Multi-Omics Era**. *Journal of Chemical Information and Modeling*, volume 60, pages 2424–2429. American Chemical Society, 2020.

2017 **Caitlyn L McCafferty** and Yuri V Sergeev. **Global computational mutagenesis provides a critical stability framework in protein structures**. *PloS one*, volume 12, page e0189064. Public Library of Science San Francisco, CA USA, 2017.

2016 **Caitlyn L McCafferty** and Yuri V Sergeev. **In silico mapping of protein unfolding mutations for inherited disease**. *Scientific Reports*, volume 6, pages 1–12. Nature Publishing Group, 2016.

2016 **Caitlyn L McCafferty** and Yuri V Sergeev. **Dataset of eye disease-related proteins analyzed using the unfolding mutation screen**. *Scientific data*, volume 3, pages 1–10. Nature Publishing Group, 2016.

2014 Jasmin C Athas, Kelly Jun, **Caitlyn McCafferty**, Olasehinde Owoseni, Vijay T John, and Srinivasa R Raghavan. **An effective dispersant for oil spills based on food-grade amphiphiles**. *Langmuir*, volume 30, pages 9285–9294. ACS Publications, 2014.

Research Experience

Postdoctoral Researcher, University of Basel, Biozentrum

February,2023 – present

In situ structural studies of motile cilia and chloroplasts.

XL/MS of intact algae cells to investigate photosynthesis across red, brown, green, and blue lineages. Cryo-ET and XL/MS of *C. reinhardtii* chloroplast for high-throughput averaging and modeling of protein complexes. Cryo-ET and XL/MS of mammalian, *C. reinhardtii*, and *S. rosetta* cilia to investigate the molecular architecture of the transition zone.

Advisor : **Dr. Benjamin D. Engel**, *Professor, Biozentrum*, University of Basel (*Lab Web-page*)

Graduate Student, University of Texas, Austin

September,2017 – December,2023

Computational prediction and assembly of protein-protein complexes.

Developed a methodology for in situ XL/MS of *Tetrahymena thermophila* mapping the ciliary interactome. Integrated AI structure prediction, XL/MS, and cryo-ET to model the Intraflagellar A complex. Assembled structural models of human red blood cell erythrocyte membrane complexes using chemical crosslink data in combination with annotated transmembrane regions. Developed a cutoff criteria for intermolecular evolutionary couplings and incorporated the couplings into the *Integrative Modeling Platform* to model individual crystal structures into low- to medium-resolution EM maps. Designed an approach to predict protein-protein interaction interfaces based on complementary surface properties, *MorphProt*.

Advisor : **Dr. Edward M. Marcotte**, *Professor, Molecular Biosciences, College of Natural Sciences*, University of Texas, Austin (*Lab Web-page*)

February,2018 – December,2023

Citizen science video game for assembling protein complexes from native extracts.

Built citizen science video game, "Protein Puzzles", for assembling protein complex structures combining multi-resolution data such as cryo-EM maps, transmembrane regions, chemical crosslinks, evolutionary couplings, and complementary surfaces. Collected and processed negative stain and cryo-EM data sets of native ciliary complexes from *Tetrahymena thermophila*.

Advisor : **Dr. David W. Taylor**, *Associate Professor, Molecular Biosciences, College of Natural Sciences*, University of Texas, Austin (*Lab Web-page*)

Postbaccalaureate Fellow, National Institutes of Health, Bethesda, Maryland

June,2015 – July,2017

Prediction of misfolding mutations and their relation to disease.

Created the Unfolding Mutation Screen (UMS), an in-silico mutagenesis technique that calculates unfolding propensities of all possible missense mutations that can occur in a protein structure, identifies critical residues to protein folding, and presents data in a series of interactive maps. Utilized UMS to understand how missense mutations affect protein folding in eye disease phenotype and enzymatic activity. Prepared a website to store data for proteins analyzed using UMS that can be accessed by clinicians, pharmacologists, and biochemists. Designed a program to test the quality of homology models based on thermodynamic stability. Developed a program for protein design based on conserving critical residues and applying feasible combinations of substitutions. The protein design program is ideal to create stabilized structures with enhanced activity, restabilize mutant structures, or provide a template to design protein-like therapeutics.

Advisor : **Dr. Yuri V. Sergeev**, *Group Leader, Protein Biochemistry & Molecular Modeling*, National Eye Institute, Bethesda (*Group Web-page*)

Intern, January,2015 – May,2015

Assessment of label-free quantification mass spectrometry tools.

Performed bioinformatics analysis on various Mass Spectrometry proteomic data using MaxQuant program and compared results to various methods of analysis. Determined a dynamic range of calculations against controls such as difference of fit, variability, and differences in normal distribution using R. Concluded the most effective Mass Spectrometry programs to be used depending on the sample and purpose.

Advisor : **Dr. Robert Hohman**, *Associate Director for Research Technologies, Research Technologies Branch*, National Institute of Allergy and Infectious Diseases, Bethesda

Fellowships & Awards

2024 ***Swiss Postdoctoral Fellowship***, Swiss National Science Foundation.

2023 ***Outstanding Research Paper Award***, University of Texas, Austin.

2022 ***Protein Society Travel Award*** from the Protein Society to attend the **Protein Society Annual Symposium** in San Francisco, CA.

2022 ***Best Talk Award*** at **The Biology of Cilia and Flagella Meeting** in Tucson, AZ.

2022 ***FEBS Transcontinental Youth Travel Fund*** from the FEBS organizing committee to attend the **Lost in Integration - Probing Biomolecules with Electrons, Photons, Neutrons and Magnetic Spins course** in Spetses, Greece.

2021 ***Marion Elizabeth Eason Endowed Scholarship,*** University of Texas, Austin.

2019 – 2022 ***NSF Graduate Research Fellowship Programs,*** National Science Foundation.

2019 – 2022 ***Dean's Prestigious Fellowship,*** University of Texas, Austin.

2019 ***Graduate School Summer Fellowship,*** University of Texas, Austin.

2019 ***Travel Award*** from the University of Texas to attend the **Three-Dimensional Electron Microscopy** meeting in Hong Kong from 8^{th} June to 14^{th} June 2019.

2016 ***Focus on Fellows Travel Grant*** awarded for best talk at the **Focus on Fellows Meeting**, National Eye Institute, Bethesda, Maryland.

2016 ***Travel Award*** from the Association for Research in Ophthalmology to attend the **ARVO Annual Meeting** meeting in Seattle, Washington in May 2016.

2016 ***Outstanding Poster Award*** awarded for best poster at the **Postbac Poster Day**, National Institutes of Health, Bethesda, Maryland.

Conferences & Presentations

2025 **McCafferty, C. L.,** Hoogerbrugge, G., Papoulas, O., Schiltz, J., Taylor, D. W., Marcotte, E. M., & Engel, B. D. "The CAGE complex: a hollow, megadalton, protein assembly in prokaryotic and eukaryotic microbes." Best poster prize at the ***EPFL Latsis Symposium***. Lausanne, Switzerland.

2025 **McCafferty, C. L.,** Papoulas, O., van den Hoek, H., Righetto, R., Van der Stappen, P., Wallingford, J.B., Marcotte, E. M., & Engel, B. D. "Explorations with cryo-ET, AI structure prediction, and XL/MS to reveal the molecular components of motile cilia." Selected talk at the ***EMBL In situ Structural Biology Workshop***. Heidelberg, Germany.

2024 **McCafferty, C. L.,** Papoulas, O., van den Hoek, H., Righetto, R., Van der Stappen, P., Wallingford, J.B., Marcotte, E. M., & Engel, B. D. "Cryo-ET, structure prediction, and XL/MS reveal the molecular components of motile cilia." Invited talk for the ***Princeton Structural Biology Colloquium***. Princeton, USA.

2024 **McCafferty, C. L.,** Papoulas, O., van den Hoek, H., Righetto, R., Van der Stappen, P., Wallingford, J.B., Marcotte, E. M., & Engel, B. D. "Cryo-ET, structure prediction, and XL/MS reveal the molecular components of motile cilia." Invited talk at the ***7th cryoNET Symposium***. Aarhus, Denmark.

2024 **McCafferty, C. L.** & Engel, B.D. "Cross-linking mass spectrometry (XL/MS) to investigate protein interaction networks of photosynthetic machinery." Poster and selected flash talk at the ***International Symposium on Photosynthesis Research***. Turku, Finland.

2024 **McCafferty, C. L.,** Papoulas, O., van den Hoek, H., Righetto, R., Van der Stappen, PP., Wallingford, J.B., Marcotte, E. M., & Engel, B. D. "Exploring Molecular Mysteries Combining Structural Methods." Invited talk for the ***Human Technopole Structural Biology Colloquium***. Milan, Italy.

2024 **McCafferty, C. L.,** van den Hoek, H., Righetto, R., Van der Stappen, P., & Engel, B.D. "In Situ Structural Insights into the Base of Mammalian Cilia." Poster presentation at the ***Three-Dimensional Electron Microscopy GRS & GRC***. Barcelona, Spain.

2024 **McCafferty, C. L.,** Papoulas, O., van den Hoek, H., Righetto, R., Van der Stappen, P., Wallingford, J.B., Marcotte, E. M., & Engel, B. D. "Visual Proteomics of Mammalian Cilia." Invited talk at the ***The Biology of Cilia and Flagella Meeting***. St. Paul, MN.

2023 **McCafferty, C. L.,** Papoulas, O., Hoogerbrugge, G., Wallingford, J.B., & Marcotte, E. M. "Combining AI structure prediction, mass spectrometry and cryo-EM to unlock the mysteries of motile cilia." Selected talk at the ***EMBL Computational Structural Biology Course***. Heidelberg, DE.

2022 **McCafferty, C. L.,** Papoulas, O., Hoogerbrugge, G.,Taylor, D. W., Wallingford, J.B., & Marcotte, E. M. "An integrative approach reveals elusive ciliary complexes and transient interactions." Poster and selected talk at the ***Protein Society Annual Symposium***. San Francisco, CA.

2022 **McCafferty, C. L.,** Papoulas, O., Hoogerbrugge, G.,Taylor, D. W., Wallingford, J.B., & Marcotte, E. M. "Structural proteomics for elusive ciliary protein complexes and transient interactions." Poster and selected talk at the ***The Biology of Cilia and Flagella Meeting***. Tucson, AZ.

2022 **McCafferty, C. L.,** Papoulas, O., Hoogerbrugge, G.,Taylor, D. W., Wallingford, J.B., & Marcotte, E. M. "Structural proteomics for studying native ciliary complexes." Poster and selected talk at the ***Three-Dimensional Electron Microscopy GRS & GRC***. Barcelona, Spain.

2022 **McCafferty, C. L.,** Papoulas, O., Jordan, M., Hoogerbrugge, G., Nichols, C., Pigino, G., Taylor, D. W., Wallingford, J.B., & Marcotte, E. M. "An integrative approach to modeling the IFT-A complex." Poster at the ***Lost in Integration - Probing Biomolecules with Electrons, Photons, Neutrons and Magnetic Spins course***. Spetses, Greece.

2022 **McCafferty, C. L.** "Structural proteomics in context." Talk at ***BioTACOs: Biology Talks About Computers, Organisms, and Systems***. University of Texas, Austin.

2019 **McCafferty, C. L.** "Protein puzzles for assembling protein structures in heterogeneous mixtures." Selected talk at the ***Women in Computational Biology Conference***. Janelia Research Campus, Ashburn, Va.

2019 **McCafferty, C. L.** "Simplified geometric representations of complementarity on interaction interfaces." Talk at ***BioTACOs: Biology Talks About Computers, Organisms, and Systems***. University of Texas, Austin.

2019 **McCafferty, C. L.,** Marcotte, E. M., & Taylor, D. W. "Classifying surfaces to assemble large macromolecular machines." Poster at the ***Three Dimensional Electron Microscopy***. Gordon Research Conference, Hong Kong.

2017 **McCafferty, C. L.** & Sergeev, Y. V. "Critical residues provide a frame for stable protein structure." Poster at ***Postbac Poster Day***. National Institutes of Health, Bethesda, MD.

2017 **McCafferty, C. L.** & Sergeev, Y. V. "A database for inherited eye disease-related proteins analyzed using the Unfolding Mutation Screen (UMS)." Poster at ***ARVO-Asia***. Brisbane, Australia.

2016 **McCafferty, C. L.** & Sergeev, Y. V. "Unfolding Mutation Screen (UMS): Insight into missense mutations and protein stability." Best graduate student and postbac talk at ***Focus on Fellows***. National Eye Institute, Bethesda, MD.

2016 **McCafferty, C. L.** & Sergeev, Y. V. "Unfolding mutation screen for inherited eye disease." Poster at ***ARVO Annual Meeting***. Seattle, WA.

2016 **McCafferty, C. L.** & Sergeev, Y. V. "Using in-silico mutagenesis to understand the role of protein folding in inherited eye disease." Outstanding poster award at ***Postbac Poster Day***. National Institutes of Health, Bethesda, MD.

Science Communication

January,2019-2022 **BioTACOS: Biology Talks About Computers, Organisms, and Systems**, Lecture Series Organizer, University of Texas, Austin.

April,2019-March,2020 **They Blinded me with Science**, Radio DJ Host, KVRX 97.1, University of Texas, Austin.

November,2016 **Girls Get Science**, Panelist and speaker, Bethesda Elementary School, Maryland.

Teaching Experience

Fall, 2024 : **Structural Biology Block Course**, Organizer and Lecturer, Biozentrum, University of Basel.

Spring, 2022 : **BCH394P: Systems Biology and Bioinformatics**, Guest Lecturer, University of Texas, Austin.

Spring, 2021 : **BCH394P: Systems Biology and Bioinformatics**, Guest Lecturer, University of Texas, Austin.

Fall, 2020 : **BCH370: Physical Methods for Biochemistry**, Supervised Teacher, University of Texas, Austin.

Fall, 2019 : **BCH370: Physical Methods for Biochemistry**, Supervised Teacher, University of Texas, Austin.

Spring, 2019 : **BCH394P: Systems Biology and Bioinformatics**, Teaching Assistant, University of Texas, Austin.

Fall, 2018 : **BCH399M: Structure and Function of Molecular Machines**, Teaching Assistant, University of Texas, Austin.

Fall, 2016 : **BIOF309: Introduction to Python**, Teaching Assistant, Foundation for Advanced Education in the Sciences, Bethesda, Maryland.

Fall, 2016 : **BIO475: New Technologies in Data Science**, Teaching Assistant, Foundation for Advanced Education in the Sciences, Bethesda, Maryland.

Supervision

Current: **Daniil Litvinov**, PhD Student, Biozentrum, University of Basel.

Current: **Jaquot Schlitz**, Masters Student, Biozentrum, University of Basel.

2025: **Benjamin Le Blanc**, Summer Intern, Biozentrum, University of Basel, Current: Masters Student, Université de Toulouse.

2024-2025: **Simon Zuffrey**, Masters Student, Biozentrum, University of Basel, Current: PhD Student, Biozentrum, University of Basel.

2024: **Lovisa Jonsson**, Summer Intern, Biozentrum, University of Basel, Current: Masters Student, University of Cambridge.

2024: **Luka Durricic**, High School Intern, Biozentrum, University of Basel.

2023: **Andrea Cocut**, Summer Intern, Biozentrum, University of Basel, Current: Masters Student, University of Zagreb.

2019-2022: **Gabriel Hoogerbrugge**, Bachelors Student, Molecular Biosciences, University of Texas, Austin, Current: PhD Student, Molecular Biosciences, University of Texas, Austin.

2019-2021: **Candice Nichols**, Bachelors Student, Molecular Biosciences, University of Texas, Austin, Current: PhD Student, Molecular Biosciences, University of Texas, Austin.

Service

2023 & 2024 **Biozentrum Research Summer**, *Mentor*, University of Basel.

2020 **Fall Undergraduate Research Symposium**, *Moderator*, University of Texas, Austin.

2018 & 2019 **Lee Elementary Science Fair**, *Judge*, Austin, TX.

2018 **Summer Undergraduate Program for Experiential Research**, *Mentor*, University of Texas, Austin.

2016 **Children's Inn**, *Volunteer*, National Institutes of Health, Bethesda, MD.

2016 **High School Scientific Training and Enrichment Program**, *Volunteer*, National Institutes of Health, Bethesda, MD.

Referees

Dr. Edward M. Marcotte
Professor, Molecular Biosciences
College of Natural Sciences
University of Texas, Austin
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Dr. John B. Wallingford
Professor, Molecular Biosciences
College of Natural Sciences
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Dr. Benjamin D. Engel
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