

Benjamin A. Neely, Ph.D.

Curriculum Vitae – May 2023

Personal Information:

Research Chemist
Biochemical and Exposure Sciences Group
Chemical Sciences Division
Material Measurement Laboratory
National Institute of Standards and Technology
NIST Charleston
Hollings Marine Laboratory
Charleston, South Carolina
United States

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Research Interests:

- Working with researchers, veterinarians, and genome sequencing labs to generate high-quality genome assemblies, and when possible, secondary RNA evidence to facilitate genome annotation. The end goal is to provide an accurate search space to underpin proteomic efforts.
- Emerging proteomic applications, specifically working with stakeholders to optimize and standardize methods for data-independent acquisition and metaproteomic analysis, with specific goals to scale to thousands of samples. These methods are crucial to human and wildlife surveillance, molecular epidemiology, biomarker discovery and microbiome characterization.
- Generating standardized proteomic data across non-model species as part of the CoMPARe Program (Comparative Mammalian Proteome Aggregator Resource), which also requires extensive genomic sequencing and annotation.
- Development of new materials for *omic applications.
- Design and improve quality controls (samples or spike-ins) and/or quality metrics useful for large-scale proteomic workflows.

Education:

The University of Georgia
B.S.E.S., Environmental Soil Science, December 2003

Medical University of South Carolina
Ph.D., Biomedical Sciences (Focus: Microbiology), September 2009

Work Experience:

- 5/16 – present Research Chemist, Chemical Sciences Division, National Institute of Standards and Technology, NIST Charleston, Charleston, SC
- 12/18 – present Research Adjunct faculty member in the College of Charleston's Graduate Program in Marine Biology (GPMB).
- 11/12 – 5/16 Staff Scientist, Director of Computational Proteomics and Bioinformatics at the MUSC Proteomics Center, Department of Pharmacology, Medical University of South Carolina, Charleston, SC
- 1/10 – 11/12 Post-Doctoral Scholar, Nephrology Proteomics Laboratory, Division of Nephrology, Department of Medicine, Medical University of South Carolina, Charleston, SC
- 8/04 – 9/09 Graduate Research Assistant, Hollings Marine Laboratory Marine Biomedical and Environmental Science Center, Medical University of South Carolina, Charleston, SC
- 5/03 – 9/03 Research Assistant, The University of Florida, Gainesville, FL
- 9/02 – 8/04 Teacher Assistant and Laboratory Technician, Crop and Soil Science Department, The University of Georgia, Athens, GA
- 6/02 – 9/02 Horticulture Exchange Student, Boomkwekerij Togtema; Buitenpost, Netherlands
- 10/01–11/01 Volunteer Intern, USDA, NRCS, Louisiana State Soil Survey, Ringgold, LA
- 5/01 – 9/01 Laboratory Technician, Department of Biochemistry, Vanderbilt University, Nashville, TN
- 5/99 – 9/99 Roving Interpreter, Tennessee Wildlife Center, Chattanooga, TN

Professional Memberships, Editorial Assignments, and Committees:

Memberships:

The Association of Biomolecular Resource Facilities (ABRF)

Committee memberships:

Proteomics Standards Research Group (ABRF), Chair

Proteomics Research Group (ABRF), Co-Chair

Steering Committee for Ocean Carbon & Biogeochemistry study (at WHOI, NSF funded)

Viral Emergence Research Initiative (The Verena Consortium)

Editorial assignments:

Editorial Advisory Board for the *Journal of Proteome Research*

Editorial Board for the *Journal of Biomolecular Techniques*

Editor for Data Independent Acquisition Methods, MassSpectrometryMethods.org

Publications:

1. Podust LM, Kim Y, Arase M, Neely BA, Beck BJ, Bach H, Sherman DH, Lamb DC, Kelly SL, Waterman MR. 2003. The 1.92-Å structure of *Streptomyces coelicolor* A3(2) CYP154C1. A new monooxygenase that functionalizes macrolide ring systems. *J Biol Chem* 278(14):12214-21.
2. Van Nostrand JD, Khijniak TJ, Neely BA, Sattar MA, Sowder AG, Mills G, Bertsch PM, Morris PJ. 2007. Reduction of nickel and uranium toxicity and enhanced trichloroethylene degradation

to *Burkholderia vietnamiensis* PR1301 with hydroxyapatite amendment. *Environ Sci Technol* 41(6):1877-82.

3. Van Nostrand JD, Arthur JM, Kilpatrick LE, **Neely BA**, Bertsch PM, Morris PJ. 2008. Changes in protein expression in *Burkholderia vietnamiensis* PR1301 at pH 5 and 7 with and without nickel. *Microbiol* 154(12):3813-24.
4. **Neely BA**, Soper JL, Greig DJ, Carlin KP, Favre EG, Gulland FM, Almeida JS, Janech MG. 2012. Serum profiling by MALDI-TOF mass spectrometry as a diagnostic tool for domoic acid toxicosis in California sea lions. *Proteome Sci* 10(1):18.
5. Korrapati MC, Shaner BE, **Neely BA**, Alge JL, Arthur JM, Schnellmann RG. 2012. Diabetes-induced renal injury in rats is attenuated by suramin. *J Pharmacol Exp Ther* 343(1):34-43.
6. Alge JL, Karakala N, **Neely BA**, Janech MG, Tumlin JA, Chawla LS, Shaw AD, Arthur JM, SAKInet Investigators. 2013. Urinary angiotensinogen and risk of severe AKI. *Clin J Am Soc Nephrol* 8(2):184-93.
7. Bhensdadia NM, Hunt KJ, Lopes-Virella MF, Michael Tucker J, Mataria MR, Alge JL, **Neely BA**, Janech MG, Arthur JM. 2013. Urine haptoglobin levels predict early renal functional decline in patients with type 2 diabetes. *Kidney Int* 83:1136-1143.
8. Alge JL, Karakala N, **Neely BA**, Janech MG, Valez JC, Arthur JM, SAKInet Investigators. 2013. Urinary angiotensinogen predicts adverse outcomes among acute kidney injury patients in the intensive care unit. *Crit Care* 17(2):R69.
9. Roper S, Zemskova M, **Neely BA**, Martin A, Gao P, Jones EE, Kraft AS, Drake RR. 2013. Targeted glycoprotein enrichment and identification in stromal cell secretomes using azido sugar metabolic labeling. *Proteomics Clin Appl* 7(5-6):367-71.
10. Arthur JM, Hill EG, Alge JL, Lewis EC, **Neely BA**, Janech MG, Tumlin JA, Chawla LS, Shaw AD. 2013. Evaluation of 32 urine biomarkers to predict progression of AKI after cardiac surgery. *Kidney Int* 85(2):431-8.
11. Alge JL, Karakala N, **Neely BA**, Janech MG, Tumlin JA, Chawla LS, Shaw AD, Arthur JM. 2013. Association of elevated urinary concentration of renin-angiotensin system components and severe AKI. *Clin J Am Soc Nephrol* 8(12):2043-52.
12. Venn-Watson S, Smith CR, Stevenson S, Parry C, Daniels R, Jensen E, Cendejas V, Balmer B, Janech M, **Neely BA**, Wells R. 2013. Blood-based indicators of insulin resistance and metabolic syndrome in bottlenose dolphins (*Tursiops truncatus*). *Front Endocrinol* 4:136.
13. **Neely BA**, Carlin KP, Arthur JM, McFee WE, Janech MG. 2013. Ratiometric measurements of adiponectin by mass spectrometry in bottlenose dolphins (*Tursiops truncatus*) with iron overload reveal an association with insulin resistance and glucagon. *Front Endocrinol* 4:132.
14. Jones EE, Powers TW, **Neely BA**, Cazares LH, Troyer DA, Parker AS, Drake RR. 2014. MALDI imaging mass spectrometry profiling of proteins and lipids in clear cell renal cell carcinoma. *Proteomics* 14:924-35.
15. Powers TW, **Neely BA**, Shao Y, Tang H, Troyer DA, Mehta AS, Haab BB, Drake RR. 2014. MALDI imaging mass spectrometry profiling of N-glycans in formalin-fixed paraffin embedded clinical tissue blocks and tissue microarrays. *PLoS ONE* 9:e106255.
16. **Neely BA**, Ferrante JA, Chaves JM, Soper JL, Almeida JS, Arthur JM, Gulland FMD, Janech MG. 2014. Proteomic analysis of plasma from California sea lions (*Zalophus californianus*)

reveals apolipoprotein E as a candidate biomarker of chronic domoic acid toxicosis. *PLoS One* 10(4):e0123295.

17. Hobeika L, Hunt KJ, **Neely BA**, Arthur JM. 2015. Comparison of the rate of renal function decline in non-proteinuric patients with and without diabetes. *Am J Med Sci* 350(6):447-52.
18. **Neely BA**, Soper JL, Gulland FMD, Bell PD, Kindy M, Arthur JM, Janech MG. 2015. Proteomic analysis of cerebrospinal fluid in California sea lions (*Zalophus californianus*) with domoic acid toxicosis identifies proteins associated with neurodegeneration. *Proteomics* 15(23-24):4051-63.
19. Pehar M, Ball LE, Sharma DR, Harlan BA, Comte-Walters S, **Neely BA**, Vargas MR. 2015. Changes in protein expression and lysine acetylation induced by decreased glutathione levels in astrocytes. *Mol Cell Proteomics* 15(2):493-505.
20. **Neely BA**, Wilkins CE, Marlow LA, Malyarenko D, Kim Y, Ignatchenko A, Sasinowska A, Sasinowski M, Nyalwidhe JO, Kislinger K, Copland JA, Drake RR. 2016. Proteotranscriptomic analysis reveals stage specific changes in the molecular landscape of clear-cell renal cell carcinoma. *PLoS ONE* 11(4):e0154074.
21. Shao S, **Neely BA**, Kao T, Eckhaus J, Bourgeois J, Brooks J, Jones JJ, Drake RR, Zhu K. 2017. Proteomic profiling of serial pre-diagnostic serum samples for early detection of colon cancer in the U.S. military. *Cancer Epidemiol Biomarkers Prev* 26(5): 711-718.
22. Zambrano JN, **Neely BA**, Yeh ES. 2017. Hormonally up-regulated neu-associated kinase: A novel target for breast cancer progression. *Pharmacol Res* 119:188-194.
23. **Neely BA**, Anderson PE. 2017. Complementary domain prioritization: A method to improve biologically relevant detection in multi-omic data sets. Proceedings of the 10th International Joint Conference on Biomedical Engineering Systems and Technologies - Volume 3: *BIOINFORMATICS* 3:68-80.
24. Mulligan JK, Patel K, Williamson T, Reaves N, Carroll W, Stephenson SE, Gao P, Drake RR, **Neely BA**, Tomlinson S, Schlosser RJ, Atkinson C. 2018. C3a receptor antagonism as a novel therapeutic target for chronic rhinosinusitis. *Mucosal Immunol* 11(5):1375-1385.
25. **Neely BA**, Prager KC, Bland AM, Fontaine C, Gulland FM, Janech MG. 2018. Proteomic analysis of urine from California sea lions (*Zalophus californianus*): a resource for urinary biomarker discovery. bioRxiv doi:10.1101/336867. *J Prot Res* 17(9):3281-3291.
26. Saito MA, Bertrand EM, Duffy ME, Gaylord DA, Held NA, Hervey WJ, Hettich RL, Jagtap P, Janech MG, Kinkade DB, Leary D, McIlvin M, Moore E, Morris R, **Neely BA**, Nunn B, Saunders JK, Shepherd A, Symmonds N, Walsh D. 2019. Progress and challenges in ocean metaproteomics and proposed best practices for data sharing. *J Prot Res* 18(4):1461-1476.
27. Davis WC, Kilpatrick LE, Ellisor DE, **Neely BA**. 2019. Characterization of a human liver NIST reference material fit for proteomics applications. *Sci Data* 6(324).
28. Heck M, **Neely BA**. 2020. Proteomics in non-model organisms: A new analytical frontier. *J Prot Res* 19(9):3595-3606.
29. **Neely BA**. 2021. Cloudy with a chance of peptides: accessibility, scalability and reproducibility with cloud-hosted environments. *J Prot Res* 20(4): 2076–2082.
30. **Neely BA**, Janech MG, Fenton MG, Simmons NB, Bland AM, Becker DJ. 2021. Surveying the vampire bat (*Desmodus rotundus*) serum proteome: a resource for identifying immunological proteins and detecting pathogens. *J Prot Res* 20(5): 2547–2559.

31. Grandal M, Hoggard M, **Neely BA**, Davis WC, Mari F. 2021. Proteogenomic assessment of intraspecific venom variability: Molecular adaptations in the venom arsenal of *Conus purpurascens*. *Mol Cell Proteomics* 20:100100.
32. Peart CR, Williams C, Pophaly SD, **Neely BA**, Gulland FMD, Adams DJ, Ng BL, Cheng W, Goebel ME, Fedrigo O, Haase B, Mountcastle J, Functammasan A, Formenti G, Collins J, Wood J, Sims Y, Torrance J, Tracey A, Howe K, Rhie A, Hoffman JI, Johnson J, Jarvis ED, Breen M, Wolf JBW. 2021. Hi-C scaffolded short- and long-read genome assemblies of the California sea lion are broadly consistent for syntenic inference across 45 million years of evolution. *Mol Ecol Res* 21, 2455–2470.
33. Khudyakov JI, Treat MD, Shanafelt MC, Deyarmin JS, **Neely BA**, van Breukelen F. 2021. Liver proteome response to torpor in a basoendothermic mammal, *Tenrec ecaudatus*, provides insights into the evolution of homeothermy. *Am J Physiol Regul Integr Comp Physiol*. 321(4):R614-R624.
34. **Neely BA** and Palmblad M. 2021. Rewinding the molecular clock: looking at pioneering molecular phylogenetics experiments in the light of proteomics. *J Prot Res* 20(10):4640-4645.
35. Albery GF, Becker DJ, Brierley L, Brook CE, Christofferson RC, Cohen LE, Dallas TA, Eskew EA, Fagre A, Farrell MJ, Glennon E, Guth S, Joseph MB, Mollentze N, **Neely BA**, Poisot T, Rasmussen AL, Ryan SJ, Seifert S, Sjodin AR, Sorrell EM, Carlson CJ. 2021. The science of the host-virus network. *Nat Microbiol* 6(12):1483-1492.
36. Becker DJ, Lei GS, Janech MG, Bland AM, Fenton MB, Simmons NB, Relich RF, **Neely BA**. 2022. Serum proteomics identifies immune pathways and candidate biomarkers of coronavirus infection in wild vampire bats. *Front Virol* 2(862961):1-13.
37. Marissen R, Varunjikar M, Laros J, Rasinger J, Neely BA, Palmblad M. 2022. compareMS2 2.0: An Improved Software for Comparing Tandem Mass Spectrometry Datasets. *J Prot Res* 22(2): 514–519.
38. Pegg CL, Schulz BL, Neely BA, Albery GF, Carlson CJ. 2022. Glycosylation and the global virome. *Mol Ecol* 00:1–8 (2022).
39. Rehfeldt TG, Gabriels R, Bouwmeester R, Gessulat S, Neely BA, Palmblad M, Perez-Riverol Y, Schmidt T, Vizcaíno JA, Deutsch EW. 2023. ProteomicsML: An Online Platform for Community-Curated Data sets and Tutorials for Machine Learning in Proteomics. *J Prot Res* 22(2):632-636.
40. Neely BA, Dorfer V, Martens L, Bludau I, Bouwmeester R, Degroevé S, Deutsch EW, Gessulat S, Käll L, Palczynski P, Payne SH, Rehfeldt TG, Schmidt T, Schwämmle V, Uszkoreit J, Vizcaíno JA, Wilhelm M, Palmblad M. 2023. Toward an Integrated Machine Learning Model of a Proteomics Experiment. *J Prot Res* 22(3):681-696.

Preprints (unpublished):

1. **Neely BA**, Ellisor DL, Davis WL. 2018. Proteomics as a metrological tool to evaluate genome annotation accuracy following de novo genome assembly: a case study using the Atlantic bottlenose dolphin (*Tursiops truncatus*). bioRxiv doi:10.1101/254250.

2. Orsburn BC, Jenkins C, Miller SM, **Neely BA**, Bumpus NN. 2020. *In silico* approach toward the identification of unique peptides from viral protein infection: Application to COVID-19. bioRxiv doi: 10.1101/2020.03.08.980383. (*in review*)
3. **Neely BA**, Stemmer PM, Searle BC, Herring LE, Martin L, Midha MK, Phinney BS, Shan B, Palmblad M, Wang Y, Jagtap PD, Kirkpatrick J. 2020. 2019 Association of Biomolecular Resource Facilities Multi-Laboratory Data-Independent Acquisition Study. bioRxiv doi:10.1101/2020.11.20.391300. (*in review*)

Selected National/International Oral Presentations:

Benjamin Neely. Extending proteomics to marine mammals: past, present and future. Institute for Marine Research (Havforskningsinstituttet). Bergen, Norway. March 11, 2022.

Benjamin Neely. Interdisciplinary perspective on Proteomes of Organisms, Organs, Tissues and Cells. Proteomics and Machine Learning Lorentz Center workshop. Leiden, Netherland. March 14, 2022.

Benjamin Neely. Exploring the protein landscape in non-model systems: insights into potential host-virus interactions and disease resistance. London Proteomics Discussion Group 10th Webinar. August 7, 2020.

Benjamin Neely. Sea lions and bats and humans, oh my! How to explore mammalian serum proteomes. Washington-Baltimore Mass Spectrometry Discussion Group April 2020 Virtual Meeting. April 20, 2020.

Benjamin Neely. Data Independent Acquisition (DIA) in the Core Facility: Practical Examples with Serum. Institutional Development Award (IDeA) National Resource for Proteomics 2020 Symposium for Core Directors and Staff. January 29, 2020. Little Rock, AR.

Benjamin Neely, Magnus Palmblad. QC Benchmark: a streamlined web application to comprehensively evaluate instrument performance and direct troubleshooting. ASMS Annual Conference, June 4, 2019, Atlanta, GA.

Benjamin Neely. Database searching in systems without a genome: lessons learned with the California sea lion. Matrix Science ASMS User Meetings. ASMS Annual Conference, June 3, 2019, Atlanta, GA.

Benjamin Neely. Standard Reference/Research Materials to assist in quality and normalization. Visualization, Comparison and Accessibility of Large Data Sets - ASMS Analytical Lab Managers workshop. ASMS Annual Conference, June 4, 2019, Atlanta, GA.

ABRF Satellite workshop: Data Independent Acquisition in Practice: Foundations and Resources for Implementing DIA. March 23, 2019. ABRF Annual Meeting, 2019, San Antonio, TX.

Y Wang, A Chien, LE Herring, PD Jagtap, L Martin, **BA Neely**, BS Phinney, P Shan, PM Stemmer. ABRF PRG Pilot Study to evaluate data-independent acquisition for protein quantification in core facility settings. ABRF Annual Meeting, 2018, Myrtle Beach, SC.

NIST and Metaproteomics. Best Practices meeting for Data Sharing of Ocean and Environmental Metaproteomics on May 3-4th of 2017. Woods Hole Oceanographic Institution, Woods Hole, MA.

BA Neely, J. Soper, F. M. D. Gulland, J. M. Arthur, M. G. Janech. Proteomic analysis of

cerebral spinal fluid from California sea lions (*Zalophus californianus*) with domoic acid toxicosis. 43rd Annual IAAAM Meeting and Conference. 2012.

BA Neely, J Soper, EG Favre, FMD Gulland, JS Almeida, JM Arthur, MG Janech. An assessment of serum peptide profiling by MALDI-TOF as a diagnostic tool for domoic acid toxicosis in California sea lions. 42nd Annual IAAAM Meeting and Conference. 2011.

BA Neely, JP Shields, AG Sutter, DW Bearden, PM Bertsch, PJ Morris. Microbial Growth Affects Zinc Oxide Nanoparticle Structure and Toxicity. Invited speaker to SETAC North America 28th Annual Meeting. 2007.

Honors and Distinctions:

- 2021 Rising Stars in Proteomics and Metabolomics (*J Prot Res*)
- 1st place student presentation at the 43rd Annual IAAAM Conference, 2012
- 2nd place poster at the MUSC Student Research Day, 2012
- 1st place student presentation at the 42nd Annual IAAAM Conference, 2011
- 1st place poster at Department of Medicine's 5th Annual Research Day, 2010
- 2nd place poster at 6th Annual SREL Student Research Symposium, 2006
- Presidential Scholars Program, Medical University of S.C., 2005
- Graduated Magna Cum Laude with honors, The University of Georgia, 2003
- Presidential Scholar, The University of Georgia, 2003
- Presidential Scholar, The University of Georgia, 2002
- Most Commendable Member Award, Georgia Soil Water Conservation Society, 2002
- Treasurer for the UGA chapter of the Soil and Water Conservation Society, 2002
- Dean's List, McDaniel College, 2000
- Honor's Program, McDaniel College, 1999
- Three-time All American Interscholastic Swim Team Member, 1998 – 1999
- NCAA's National Student Athlete Day Award, 1998

Scholarships and Fellowships:

- South Carolina Sea Grant Fellowship, 2008-2009
- Deans Incentive Award, Medical University of S.C., 2008, 2007
- Travel Award to SETAC North America 28th Annual Meeting, 2007
- Science to Achieve Results Fellowship, U.S. EPA, 2005-2008
- Graduate Student Assistantship, Medical University of S.C., 2004
- Georgia Plant Food Scholarship, 2003
- Dudley Mays Scholarship, The University of Georgia, 2003, 2002
- Four-year Academic Scholarship, McDaniel College, 1999

Teaching Experience:

- 2002 – 2003 Soils and Hydrology, The University of Georgia, Teaching Assistant, 3 semesters
Responsible for weekly lecture, grading, and assisting students.
- 2009 General Microbiology, College of Charleston, Laboratory Instructor, 1 semester
Responsible for weekly lecture, grading, and assisting students.
- 2010 Biodiversity, Ecology, and Conservation Biology, College of Charleston, Instructor, 1 semester.
Developed syllabus, planned lectures, designed tests, and created new and exciting projects for students.

