Sam Pellock, Ph.D.
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Research Experience

Aug 2019-Present	Postdoctoral Scholar under Prof. David Baker, University of Washington, Seattle, WA
Aug 2014-Jul 2019	Graduate Research Assistant under Prof. Matthew R. Redinbo, UNC-Chapel Hill, Chapel Hill, NC
Aug 2013-May 2014	Undergraduate Research Assistant under Prof. James R. Cox, Murray State University, Murray, KY
Jun 2013-Aug 2013	Research Internship at NASA's Student Airborne Research Program, NASA, Palmdale and Irvine, CA
Apr 2012-May 2013	National Science Foundation Biomathematics in Population Studies ($BioMaPS^2$) Undergraduate Research Program, MSU, Murray, KY

Education

University of North Carolina at Chapel Hill (Aug 2014-Jul 2019)
Research Advisor: Prof. Matthew R. Redinbo
Thesis: The Structure, Function, and Inhibition of Gut Bacterial β-Glucuronidases
Ph.D. in Chemistry

Murray State University (Aug 2010-May 2014)
Thesis Advisor: Prof. James R. Cox
Honors Thesis: The Nature of π-π Stacking Interactions in Protein-Ligand Complexes
B.S. in Chemistry/Biochemistry, Minor in Biology, *summa cum laude*, Outstanding Senior in Chemistry, Outstanding Senior Graduate

Peer-reviewed publications

1. Cross, T. L., Simpson, A. M. R., Lin, C., Hottmann, N. M., Bhatt, A. P., **Pellock, S. J.**, Nelson, E. R., Loman, B. R., Wallig, M. A., Vivas, E. I., Suchodolski, J., Redinbo, M. R., Rey, F. E., Swanson, K. S. (2024) Gut microbiome responds to alteration in female sex hormone status and exacerbates metabolic dysfunction. *Gut microbes.* 16, 1-19.
2. Sumida, K. H., Núnez-Franco, R., Kalvet, I., **Pellock, S. J.**, Wicky, B. I. M., Milles, L. F., Dauparas, J., Wang, J., Kipnis, Y., Jameson, N., Kang, A., De La Cruz, J., Sankaran, B., Bera, A. K., Jiménez-Osés, Baker, D. (2024) Improving Protein Expression, Stability, and Function with ProteinMPNN. *JACS.* 146, 2054-2061.
3. Watson, J. L., Juergens, D., Bennett, N. R., Trippe, B. L., Yim, J., Eisenach, H. E., Ahern, W., Borst, A. J., Ragotte, R. J., Milles, L. F., Wicky, B. I. M., Hanikel, N., **Pellock, S. J.**, Courbet, A., Sheffler, W., Wang, J., Venkatesh, P., Sappington, I., Vàzquez-Torres, S., Lauko, A., De Bortoli, V., Mathieu, E., Ovchinnikov, S., Barzilay, R., Jaakkola, T. S., DiMaio, F., Baek, M., Baker, D. (2023) De novo design of protein structure and function with RFdiffusion. *Nature*. 620, 1089-1100.
4. Yeh, A. H. W. Y., Norn, C., Kipnis, Y., Tischer, D., **Pellock, S. J.**, Evans, D., Ma, P., Lee, G. R., Zhang, J. Z., Anishchenko, I., Coventry, B., Cao, L., Dauparas, J., Halabiya, S., DeWitt, M., Carter, L., Houk, K. N., Baker, D. (2023) De novo design of luciferases with deep learning. *Nature*. 614, 774-780.

5. Dauparas, J., Anishchenko, I., Bennett, N., Bai, H., Ragotte, R. J., Milles, L. F., Wicky, B. I. M., Courbet, A., de Haas, R. J., Bethel, N., Leung, P. J. Y., Huddy, T. F., **Pellock, S.**, Tischer D., Chan, F., Koepnick, B., Nguyen, H., Kang, A., Sankaran, B., Bera, A. K., King, N. P., Baker. D. (2022) Robust deep learning-based protein sequence design using ProteinMPNN. *Science.* 378, 49-56.
6. Anishchenko, I.*, **Pellock, S. J.***, Chidyausiku, T. M., Ramelot, T. A., Ovchinnikov, S., Hao, J., Bafna, K., Norn, C., Kang, A., Bera, A. K., DiMaio, F., Carter, L., Chow, C. M., Montelione, G. T., Baker, D. (2021) De novo protein design by deep network hallucination. *Nature.* 600, 547-552.
7. Bhatt, A. P., **Pellock, S. J.**, Biernat, K. A., Walton, W. G., Wallace, B. D., Creekmore, B. C., Letertre, M. M., Swann, J. R., Wilson, I. D., Roques, J. R., Darr, D. B., Bailey, S. T., Montgomery, S. A., Roach, J. M., Azcarate-Peril, M. A., Sartor, R. B., Gharaibeh, R. Z., Bultman, S. J., Redinbo, M. R. (2020) Targeted inhibition of gut bacterial β-glucuronidase activity enhances anticancer drug efficacy. *Proc. Natl. Acad. Sci.* 117, 7374-738.
8. Bartolini, D., De Franco, F., Torquato, P., Marinelli, R., Cerra, B., Ronchetti, R., Schon, A., Fallarino, F., De Luca, A., Bellezza, G., Ferri, I., Sidoni, A., Walton, W. G., **Pellock, S. J.**, Redinbo, M. R., Mani, S., Pellicciari, R., Gioiello, A., Galli, F. (2020) Garcinoic Acid is a Natural and Selective Agonist of Pregnane X Receptor. *J. Med. Chem.* 63, 3701-3712.
9. Jariwala, P. B., **Pellock, S. J.**,Goldfarb, D., Cloer, E. W., Artola, M., Simpson, J. B., Bhatt, A. P., Walton, W. G., Roberts, L. R., Major, M. B., Davies, G. J., Overkleeft, H. S., Redinbo, M. R. (2019) Discovering the microbial enzymes driving drug toxicity with activity-based protein profiling. *ACS Chem. Biol. 15*, 217-225.
10. **Pellock, S. J.*#**, Walton, W. G*., Redinbo, M. R.# (2019) Selecting a single stereocenter: the molecular nuances that differentiate β-Hexuronidases in the human gut microbiome. *Biochemistry*. *58*, 1311-1317.
11. Biernat, K. A., **Pellock, S. J.**, Bhatt, A. P., Bivins, M. M., Walton, W. G., Tran, B. N. T., Wei, L., Snider, M. C., Cesmat, A.P., Tripathy, A., Erie, D. A., and Redinbo, M.R. (2019) Structure, function and inhibition of drug reactivating human gut microbial β-glucuronidases. *Sci. Rep. 9*, 825.
12. **Pellock, S. J.**, Walton, W. G., Ervin, S. M., Torres-Rivera, D., Creekmore, B. C., Bergan, G., Dunn, Z. D., Li, B., Tripathy, A., Redinbo, M. R. (2019) Discovery and characterization of FMN-binding β-glucuronidases in the human gut microbiome, *J. Mol. Biol. 431*, 970-980.
13. **Pellock, S. J.***, Walton, W. G.*, Biernat, K. A., Torres-Rivera, D., Creekmore, B. C., Xu, Y., Liu J., Tripathy, A., Stewart, L.J., Redinbo, M. R. (2018) Three structurally and functionally distinct β-glucuronidases from the human gut microbe *Bacteroides uniformis*, *J. Biol. Chem. 293*, 18559-18573.
14. **Pellock, S. J.**, Creekmore, B. C., Walton, W. G., Mehta, N., Biernat, K. A., Cesmat, A. P., Ariyarathna, Y., Dunn, Z. D., Li, B., Jin, J., James, L. I., Redinbo, M. R. (2018) Gut microbial β-glucuronidase inhibition via catalytic cycle interception, *ACS Cent. Sci. 4*, 868-879.
15. Little, M. S., **Pellock, S. J.**, Walton, W. G., Tripathy, A., Redinbo, M. R. (2018) Structural basis for the regulation of β-glucuronidase expression by human gut Enterobacteriaceae. *Proc. Natl. Acad. Sci. 115*, E152-E161.
16. Pollet, R. M., D'Agostino, E. H., Walton, W. G., Xu, Y., Little, M. S., Biernat, K. A., **Pellock, S. J.**, Patterson, L. M., Creekmore, B. C., Isenberg, H. N., Bahethi, R. R., Bhatt, A. P., Liu, J., Gharaibeh, R. Z., Redinbo, M. R. (2017) An atlas of β-glucuronidases in the human intestinal microbiome. *Structure. 25*, 967-977.

17. **Pellock, S. J.**, Redinbo, M. R. (2017) Glucuronides in the gut: sugar-driven symbioses between microbe and host. *J. Biol. Chem. 292*, 8569-8576.
18. Wallace, B. D., Roberts, A. B., Pollet, R. M., Ingle, J. D., Biernat, K. A., **Pellock, S. J.**, Venkatesh, M. K., Guthrie, L., O'Neal, S. K., Robinson, S. J., Dollinger, M., Figueroa, E., McShane, S. R., Cohen, R. D., Jin, J., Frye, S. V., Zamboni, W. C., Pepe-Ranney, C., Mani, S., Kelly, L., Redinbo, M. R. (2015) Structure and inhibition of microbiome β-glucuronidases essential to the alleviation of cancer drug toxicity. *Chem. Biol. 22*, 1238-1249.
19. Whittington, C. P., **Pellock S. J.**, Cunningham, R. L., Cox, J. R. (2014) Combining content and elements of communication into an upper-level biochemistry course. *Biochem. Mol. Biol. Educ. 42*, 136-141.
20. Copeland, K. L., **Pellock, S. J.**, Cox, J. R., Cafiero, M. L., Tschumper, G. S. (2013) Examination of tyrosine/adenine stacking interactions in protein complexes. *J. Phys. Chem. B. 117*, 14001-14008.
21. **Pellock, S.**, Thompson, A., He, K. S., Mecklin, C. J., Yang, J. (2013) Validity of Darwin's naturalization hypothesis relates to the stages of invasion. *Community Ecology*. *14*, 172-179.

***Indicates co-first author**
#Indicates co-corresponding

Preprints

1. Lee, G. R.*, **Pellock, S. J.***, Norn, C.*, Tischer, D., Dauparas, J., Anishchenko, I., Mercer, J. A. M., Kang, A., Bera, A. K., Nguyen, H., Brackenbrough, E., Sankaran, B., Goreshnik, I., Vafeados, D., Roullier, N., Han, H. L., Coventry, B., Haddox, H. K., Liu, D. R., Yeh, A.H.W., Baker, D. (2023). Small-molecule binding and sensing with a designed protein family. *Biorxiv*. https://doi.org/10.1101/2023.11.01.565201

Patents

1. U.S. Patent 61444236, "De novo designed NTF2-like scaffolds for de novo design of enzymes and small molecule binders," Jan 17, 2023
2. U.S. Patent 11339178, "Inhibitors of Microbial beta-glucuronidase enzymes and uses thereof," May 24, 2022

Awards

- Washington Research Foundation Postdoctoral Fellowship (2021-2023)
- Winner of UNC Center for Gastrointestinal Biology and Disease Research Competition (2017)
- NIH T32 UNC Biophysics Training Program Awardee (2015-2016)
- MSU Outstanding Senior (Spring 2014)
- MSU Outstanding Senior Chemistry Major (Spring 2014)
- ACS Undergraduate Award in Analytical Chemistry (Spring 2013)

Oral and Poster Presentations

- Protein design with deep learning. Invited lecture at Manchester Institute of Biotechnology, Manchester, UK. July 2023.
- De novo design of plastic-degrading enzymes. Oral presentation, Washington Research Foundation Postdoctoral Fellows Symposium, Seattle, WA. May, 2023.
- De novo design of small-molecule binding proteins with deep learning. Summer RosettaCON, Leavenworth, WA. August, 2022.

- De novo design of plastic degrading enzymes. Poster presentation, Washington Research Foundation Postdoctoral Fellows Symposium. May, 2022.
- The myriad interactions of drugs with gut bacterial β-glucuronidases. Oral Presentation, The Toxicology Forum, Alexandria, VA. July, 2019.
- A structural view of gut bacterial β-glucuronidases. Poster Presentation, Keystone Microbiome Conference, Montreal, QC. March, 2019.
- The human gut microbiota encodes a family of FMN-binding β-glucuronidases. Poster Presentation, Gordon Research Conference: Enzymes, cofactors, and metabolic pathways. Waterville Valley, NH. July, 2018.
- Gut microbial β-glucuronidase inhibition via catalytic cycle interception. Oral and Poster Presentation, Gordon Research Seminar: Enzymes, cofactors, and metabolic pathways. Waterville Valley, NH. July, 2018.
- Substrate and activity-based inhibition of gut microbial β-glucuronidases. Poster Presentation, NC microbiome consortium, Research Triangle Park, NC. May 2017.
- Substrate and activity-based inhibition of gut microbial β-glucuronidases. Poster Presentation, Keystone Microbiome Conference, Keystone, CO. February 2017.
- Substrate and activity-based inhibition of gut microbial β-glucuronidases. Oral Presentation, CGIBD research competition, Chapel Hill, NC. November 2016.
- An Investigation of Controls on Ozone Production in Southern California. Oral Presentation, NASA Student Airborne Research Program, Irvine, CA. July 2013.
- Testing Darwin's Naturalization Hypothesis using Generalized Linear Models. Poster Presentation, National Institute for Mathematical and Biological Synthesis (NIMBioS) Conference, Knoxville, TN. November 2012.

Teaching and mentoring

- Mentored four graduate students in 3-month rotation projects in the Baker lab at UW
  - Kiera Sumida
  - Cullen Demakis
  - Adam Chazin-Gray
  - Soichiro Nishio
- Mentored two graduate students in multi-year projects in the Baker lab at UW
  - Anna Lauko
  - Kiera Sumida
- Mentored two post-docs in the Baker lab at UW
  - Jason Qian
  - Andrew Hunt
- Mentored undergraduate and graduate students in the Redinbo lab at UNC-Chapel Hill
  - Ben Creekmore (undergraduate student)
  - Andrew Cesmat (undergraduate student)
  - Parth Jariwala (graduate student)
- Taught graduate level biophysics course at UNC-Chapel Hill (Fall 2017)
- Science tutor at Murray State University Athletics Department (2012-2014)