

Nicholas C. Fitzkee

Professor of Chemistry

Department of Chemistry, Mississippi State University
310 President Circle, Room 1115, Mississippi State, Mississippi, 39762

W: (662) 325-1288 H: (662) 324-7343 C: (662) 518-9530
nfitzkee@chemistry.msstate.edu or nickfitzkee@gmail.com
<http://fitzkee.chemistry.msstate.edu/>

- EDUCATION:**
- 2001-2005 **Johns Hopkins University** (Baltimore, MD)
Ph.D., Biophysics
Adviser: Dr. George D. Rose
- 1997-2001 **Carnegie Mellon University** (Pittsburgh, PA)
Bachelor of Science, Computational Physics
Minor: Biological Sciences
Graduated with University Honors
- EMPLOYMENT:**
- 2021-Present *Professor*
- 2017-2021 *Associate Professor*
- 2011-2017 *Assistant Professor*
Department of Chemistry
Mississippi State University (Starkville, MS)
- 2007-2011 *Postdoctoral Fellow* with Dr. Ad Bax
National Institute of Diabetes & Digestive & Kidney Diseases
National Institutes of Health (Bethesda, MD)
Development of NMR methodologies to study HIV-1 integrase
- 2005-2007 *Postdoctoral Fellow* with Dr. Betrand García-Moreno E.
T.C. Jenkins Department of Biophysics
Johns Hopkins University (Baltimore, MD)
Modeling electrostatic interactions in unfolded proteins
- 2001-2005 *Doctoral Student* with Dr. George D. Rose
T.C. Jenkins Department of Biophysics
Johns Hopkins University (Baltimore, MD)
Physical interactions and conformational bias in unfolded proteins
- 1998-2001 *Undergraduate Researcher* with Dr. John Rosenberg
Department of Biological Sciences
University of Pittsburgh (Pittsburgh, PA)
Crystallography and function of the EcoRI restriction enzyme

FUNDING:	2022-2025	NSF Track-2 MRI (DBI 2215258) “MRI: Acquisition of the First 800 MHz NMR with Cryoprobe in the State of Mississippi for Biological and Chemical Research and Teaching” (PI, \$3,147,269)
	2019-2024	NIH R01 (AI140985) “New Inhibitors Targeting HIV-1 Integrase During Viral Maturation” (Co-PI, \$1,700,000 total, \$185,000 to MSU)
	2018-2023	NIH R01 (AI139479): “The Structure, Orientation, and Competitive Interactions of <i>S. Epidermidis</i> Biofilm Proteins on Surfaces” (PI, \$1,800,000)
	2018-2023	NSF Project (MCB 1818090): “NMR-Based Approaches for Investigating Protein-Surface Interactions” (PI, \$650,000)
	2018-2023	NIH COBRE (P20 GM103646) in Pathogen-Host Interactions (co-PI, \$10,800,000). Graduated after receiving an independent R01.
	2017-2020	NSF REU: “Research Experience for Undergraduates: Food, Energy, and Water Security” (Co-PI, \$274,000)
	2015-2018	NIH R15 (GM113152): “Functionalized Gold Nanoconjugates: Understanding the Mechanism of Protein Binding” (PI, \$330,000)
	2014-2016	Mississippi EPSCoR Seed Grant (\$36,000)
	2013-2014	SEC Travel Award (\$2,500)
	2013-2014	MSU Cross-College Research Grant (\$2,000)
	2012-2013	Henry Family Research Foundation Grant (\$10,000)
	2010-2011	NIH Intramural AIDS Research Fellowship (full stipend support)
	2009	NIH Fellows Award for Research Excellence
	2007-2009	American Cancer Society Postdoctoral Fellowship <i>Declined because of institutional policy restrictions</i>
	2005-2007	Institute for Multiscale Modeling of Biological Interactions Postdoctoral Fellow (full stipend support)
	2001-2003	Francis D. Carlson Predoctoral Fellowship
	2000-2001	Barry M. Goldwater Undergraduate Scholarship
AWARDS:	2019	MSU Alumni Graduate Teaching Award (University Level Competition, one recipient per year)
	2019	Honors College Faculty Mentor Award (University Level Competition, one recipient per year)
	2017	MSU Dean’s Eminent Scholar
	2017	MSU College of Arts and Sciences Researcher of the Year
	2007-2009	American Cancer Society Postdoctoral Fellowship (declined)
	2005	Dean’s Teaching Fellowship, Johns Hopkins University (Introduction to Bioinformatics)
	2001	Richard E. Cutkosky Award in Physics, Carnegie Mellon University
	2000	Phi Beta Kappa

TEACHING:

At Mississippi State University (Starkville, MS):

- 2021-Present *Instructor*, General Biochemistry II (BCH 4613)
 2018-Present *Instructor*, Theory of NMR Spectroscopy (CH 8613)
 2012-Present *Instructor*, Graduate Methods in Biophysical Chemistry (CH 8613)
 2020 Certified for Distance Education Pedagogy (MSU)
 2017-2020 *Instructor*, Thermodynamics and Kinetics (CH 4413)
 2013-2018 *Instructor*, Professional Chemistry: Tools (CH 2141)
 2011-2016 *Instructor*, Introduction to Biophysical Chemistry (CH 4403)
- 2014 *Instructor*, General Chemistry I (CH 1213)
 2013 *Instructor*, Professional Chemistry: Research (CH 4141)

At other institutions:

- 2010 *Instructor and Mentor*, Community College Summer Enrichment Program (CCSEP)
 National Institutes of Health (Bethesda, MD)
 2009 *Research Mentor*, Summer Internship Program (SIP)
 National Institutes of Health (Bethesda, MD)
 2006 *Instructor*, Introduction to Bioinformatics (AS 250.265)
 Johns Hopkins University (Baltimore, MD)
 2002 *Teaching Assistant*, Proteins and Nucleic Acids (AS 250.687)
 Johns Hopkins University (Baltimore, MD)
 2001 *Teaching Assistant*, Introduction to Bioinformatics (AS 250.265)
 Johns Hopkins University (Baltimore, MD)
 2000 *Head tutor for all first-year computer science classes (15-12X)*
 Carnegie Mellon University (Pittsburgh, PA)
 1999 *Teaching Assistant*, Introduction to Programming in C++ (15-127)
 Carnegie Mellon University (Pittsburgh, PA)

SERVICE TO THE COMMUNITY:

- 2019-Present **Associate Treasurer and Website Support, Gibbs Society**
 for Biological Thermodynamics
 2021-Present Editorial Board: Review Editor for *Frontiers in Molecular Biosciences*
 2012-Present **Organizer for Regional Summer Biochemistry Boot Camp**,
 Serving students from MS, AL, and FL (NSF Funded in 2019)
 2023 Panel Review, National Science Foundation
 2022 Panel Review, National Science Foundation
 2022 NIH Study Section Ad Hoc Reviewer (BMBl, EBIT)
 2021 NIH Study Section Ad Hoc Reviewer (BMBl)
 2019-2021 Panel Review, National Science Foundation (4 panels)
 2019 Ad hoc reviewer for UKRI (United Kingdom Research and Innovation)

SERVICE TO THE COMMUNITY: (CONT.)	2019	Panel Reviewer, NSF Division of Molecular and Cellular Biosciences (Molecular Biophysics)
	2018, 2019	Ad-hoc reviewer, NSF Division of Molecular and Cellular Biosciences (Molecular Biophysics)
	2017	Ad-hoc reviewer, ACS Petroleum Research Fellowship
	2016	Co-Organizer for the 30th Gibbs Conference on Biological Thermodynamics (Carbondale, IL; http://folding.chemistry.msstate.edu/gibbs30/)
	2016	Organizer for the Ninth Annual Meeting of the Mississippi Regional Biophysical Consortium (Starkville, MS; http://folding.chemistry.msstate.edu/mrbc9/)
	2014	NIH Early-Career Reviewer (MSFB Study Section)
	2013	Ad-hoc reviewer, Louisiana State Board of Regents
	2011	Ad-hoc Reviewer, Israeli Science Foundation
	2010	Career Symposium Planning Committee National Institutes of Health (Bethesda, MD)
	Various	Reviewer for: <i>Nature Chemistry</i> , <i>Nature Communications</i> , <i>ACS Nano</i> , <i>Nanoscale</i> , <i>Small</i> , <i>Journal of the American Chemical Society</i> , <i>Journal of Biomolecular NMR</i> , <i>Langmuir</i> , <i>International Journal of Molecular Sciences</i> , <i>Proteins: Structure, Function, and Bioinformatics</i> , <i>The Journal of Physical Chemistry (Parts B and C)</i> , <i>Colloids and Surfaces</i> , <i>Analytical Biochemistry</i> , <i>Biomacromolecules</i> , <i>BBA Proteins and Proteomics</i> , <i>ACS Applied Materials and Interfaces</i> , <i>Biophysical Journal</i> , <i>Journal of Physical Chemistry Letters</i> , <i>International Journal of Biological Macromolecules</i>
SERVICE TO THE UNIVERSITY:	2021-Present	MSU University Graduate Council
	2019-Present	Treasurer, Phi Beta Kappa, Gamma of Mississippi
	2018-Present	Arts & Sciences Faculty Mentor
	2013-Present	Ad-hoc reviewer, MSU Goldwater Scholarship Competition
	2013-2018	MSU Phi Beta Kappa Application Committee Library and IT Resources Subcommittee Chair
	2011-2020	MSU Society of Scholars Committee
	2012-2018	MSU Structural Biophysics Interest Group, Founder
SERVICE TO THE DEPARTMENT:	2014-Present	Instrument Committee
	2011-Present	Graduate Affairs Committee
	2011-Present	NMR Facility Director , responsible for facility planning, overseeing instrument billing, computer security, and pulse program implementation
	2019	Search Committee Chair (Physical & Biological Chemistry); successfully recruited Dr. Chris Johnson and supported the recruitment of Dr. Kun Wang
	2014-2017	Safety Committee
	2014-2016	Departmental Seminar Coordinator

**SERVICE TO THE DEPARTMENT:
(CONT.)** 2001-2007 UNIX and Network Security Consultant
T.C. Jenkins Department of Biophysics
Johns Hopkins University (Baltimore, MD)

SOFTWARE DEVELOPMENT 2021-Present Biochemistry Boot Camp YouTube Videos and NMR instructional material (over 8,000 views)
<https://www.youtube.com/@FitzkeeLab>
2011-Present LINUS Molecular Simulation Package
<http://folding.chemistry.msstate.edu/dist/>
2005-Present The Protein Coil Library
<http://folding.chemistry.msstate.edu/coil/>

STUDENT MENTORING Since 2011, I have mentored a diverse group of:
4 postdoctoral fellows
1 foreign visiting scholar
12 Ph.D. graduate students
5 M.S. graduate students
39 undergraduate student researchers
3 high school student researchers

My postdoctoral fellows have gone on to successful industry careers at Merck and AstraZeneca, or academic careers at PUIs. My graduate students have attained postdoctoral positions at Brown, Vanderbilt, UNC Chapel Hill, and the National Institutes of Health. Many have also gone on to careers in the chemical, pharmaceutical, and medical diagnostics industries.

PUBLICATIONS:

Peer-reviewed publications. Asterisks denote undergraduate authors.

1. Peng, W.; Somarathne, R.P., Don, R.W., Scott, C.N., **Fitzkee, N.C.**, Zhang, D. (2023) "Polarized Resonance Synchronous Spectroscopy as an Informative, Sensitive, and Convenient Technique for Probing Protein Aggregations." *In preparation*.
2. Wamsley, M., Carter, K.R. Wathudura, P.D., Somarathne, R.P., **Fitzkee, N.C.**, Emerson, J.P., Zhang, D. (2023) "Amino Acid and Protein UV-vis Extinction from 320 nm to 800 nm: Optical Absorption Induced by Charge Transfer, Impurity Interferences, or Light Scattering by the Biomolecules?" *In preparation*.
3. Yadav, R.,[†] Perera, Y.R.,[†] South, T.M.,* McConnell, K.D., Chappell, E.R.,* and **Fitzkee, N.C.** (2023) "Solution Structure, Dynamics, and Surface Interaction of the Autolysin R2ab Repeat Domain of *S. epidermidis*." *In preparation*. [†] Contributed equally.
4. **Fitzkee, N.C.**, Yadav, R., Ying, J. (2022) "Experiments for Measuring RDCs in Biomolecules." Chapter 6 in *Residual Dipolar Couplings: Principles and Applications*, Lishan Yao and Beat Vogeli, eds. Royal Society of Chemistry. *Submitted*.
5. Santos-Rivera, M., **Fitzkee, N.C.**, Hill, R.A. Baird, R.E., Blair, E., Thoresen, M., Woolums, A.R., Meyer, F., and Vance, C.K. (2023) "Nuclear magnetic resonance-based metabolomics of blood plasma from dairy calves infected with the main causal agents of Bovine Respiratory Disease (BRD)." *Scientific Reports*. *Accepted*. *Preprint available at* <https://doi.org/10.21203/rs.3.rs-960865/v1>.
6. Ibrahim, A.Y., Khaodeuanepheng, N.P., Amarasekara, D.L., Correia, J.J., Lewis, K.A., **Fitzkee, N.C.**, Hough, L.E., Whitten, S.T. (2022) "Intrinsically Disordered Regions That Drive Phase Separation Form a Robustly Distinct Protein Class." *Journal of Biological Chemistry*. *In press*. <https://doi.org/10.1016/j.jbc.2022.102801>
7. Xu, J.X., Alom, M.S., Yadav, R. **Fitzkee, N.C.** (2022) "Predicting Protein Function and Orientation on a Gold Nanoparticle Surface Using a Residue-Based Affinity Scale" *Nature Communications*. *Accepted*. *Preprint available at* <https://doi.org/10.1101/2022.03.29.486298>.
8. McConnell, K.D., **Fitzkee, N.C.**, Emerson, J.P. (2022) "Metal Ion Binding Can Induce Local Unfolding in Human Carbonic Anhydrase II." *Inorganic Chemistry*. **61**: 1249-1253. <https://doi.org/10.1021/acs.inorgchem.1c03271>
9. Paiz, E.A., Allen, J.H., Correia, J.J., **Fitzkee, N.C.**, Hough, L.E., Whitten S.T. (2021) "Beta Turn Propensity and a Model Polymer Scaling Exponent Identify Disordered Proteins that Phase Separate." *Journal of Biological Chemistry* 297 (5): 101343. <https://doi.org/10.1016/j.jbc.2021.101343> Website available at <http://folding.chemistry.msstate.edu/utills/parse.html>.
10. Perera, Y.R.,[†] Xu, J.X.,[†] Amarasekara, D.L., Hughes, A.C.,* Abbood, I.,* **Fitzkee, N.C.** "Understanding the Adsorption of Peptides and Proteins

**PUBLICATIONS:
(CONT.)**

- onto PEGylated Gold Nanoparticles.” *Molecules*. (Special Issue: Protein Adsorption and Conformational Changes.) † Contributed equally
<https://doi.org/10.3390/molecules26195788>
11. Xu, J.X.,† Alom, M.S.,† **Fitzkee, N.C.** (2021) “Quantitative Measurement of Multi-Protein Nanoparticle Interactions using NMR Spectroscopy.” *Analytical Chemistry*. 93(35): 11982-11990. † Contributed equally
<https://doi.org/10.1021/acs.analchem.1c01911>
 12. Xu, J.X., **Fitzkee, N.C.** (2021) “Solution NMR of Nanoparticles in Serum: Protein Competition Influences Binding Thermodynamics and Kinetics.” *Frontiers in Physiology*. 12: 715419.
<https://doi.org/10.3389/fphys.2021.715419>
 13. Hu, Y., Park, N., Seo, K.S., Park, J., Somarathne, R.P., Olivier, A.K., **Fitzkee, N.C.**, Thornton, J.A. (2021) “Pneumococcal surface adhesion A protein (PsaA) interacts with human Annexin A2 on airway epithelial cells.” *Virulence*. 12(1): 1841-1854.
<https://doi.org/10.1080/21505594.2021.1947176>
 14. Somarathne, R.P., Chappell, E.R.,* Perera, Y.R., Yadav, R. Park, J., **Fitzkee, N.C.** (2021) “Understanding How Staphylococcal Autolysin Domains Interact with Polystyrene Surfaces.” *Frontiers in Microbiology*. 12: 658373. <https://doi.org/10.3389/fmicb.2021.658373>
 15. Tucker, L.J., Grant, C.S., Gautreaux, M.A. Amarasekara, D., **Fitzkee, N.C.**, Janorkar, A.V., Varadarajan, A., Kundu, S., Priddy, L.B.. (2021) “Physicochemical and Antimicrobial Properties of Thermosensitive Chitosan Hydrogel Loaded with Fosfomycin.” *Marine Drugs*. 19(3): 144.
<https://doi.org/10.3390/md19030144>
 16. Burcham, L.R., Hill, R.A., Caulkins, R.C., Emerson, J.P. Nanduri, B., Rosch, J.W., **Fitzkee, N.C.**, Thornton, J.A. (2020) “*Streptococcus pneumoniae* Metal Homeostasis Alters Cellular Metabolism.” *Metallomics*. 12(9): 1416-1427. <https://doi.org/10.1039/D0MT00118J>
 17. Cai, L., Lim, H., **Fitzkee, N.C.**, Cosovic, B. Jeremic, D. (2020) “Feasibility of Manufacturing Strand-Based Wood Composite Treated with β -Cyclodextrin-Boric Acid for Fungal Decay Resistance.” *Polymers*. 12 (2): 274. <https://doi.org/10.3390/polym12020274>
 18. Perera, Y.R., South, T.M.,* Hughes, A.C.,* Parkhurst, A.N.,* Williams, O.W.,* Davidson, M.B., Wilks, C.A.,*, Mlsna, D.A., **Fitzkee, N.C.** (2020) “Using NMR to Measure Protein Binding Capacity on Gold Nanoparticles.” *Journal of Chemical Education*. 97(3): 820-824.
<https://doi.org/10.1021/acs.jchemed.9b00625>
 19. Perera, Y.R., Hill, R.A., **Fitzkee, N.C.** (2019) “Protein Interactions with Nanoparticle Surfaces: Highlighting Solution NMR Techniques.” *Israel Journal of Chemistry*. 59 (11-12): 962-979.
<https://doi.org/10.1002/ijch.201900080>
 20. Hill, R.A., Hunt, J.J.* Sanders, E.,* Tran, M.,* Burk, G.A., Mlsna, T.E., **Fitzkee N.C.**, (2019) “Effect of Biochar on Microbial Growth: A Metabolomics and Bacteriological Investigation in *E. coli*.” *Environmental*

**PUBLICATIONS:
(CONT.)**

- Science & Technology*. 53 (5): 2635-2646.
<https://doi.org/10.1021/acs.est.8b05024>
21. Athukorale S., Leng X., Xu J.X., Perera Y.R., **Fitzkee N.C.**, and Zhang D. (2019) "Surface Plasmon Resonance, Formation Mechanism, and Surface Enhanced Raman Spectroscopy of Ag⁺-stained Gold Nanoparticles." *Frontiers in Chemistry – Nanoscience*. 7: 27. <https://doi.org/10.3389/fchem.2019.00027>.
 22. Jinasena D., Simmons R.*, Gyamfi, H., **Fitzkee N.C.** (2019) "Molecular Mechanism of the Pin1-Histone H1 Interaction." *Biochemistry*. 58 (6): 788-798. <https://doi.org/10.1021/acs.biochem.8b01036>
 23. Zhang, Y. Zai-Rose, V., Price, C.J.*, Ezzell, N.A.*, Bidwell III, G.L., Correia, J.J., **Fitzkee, N.C.** (2018) "Modeling the Early Stages of Phase Separation in Disordered Elastin Like Proteins." *Biophysical Journal*. 114 (7): 1563-1578. <https://doi.org/10.1016/j.bpj.2018.01.045>
 24. Yadav, D.K., Tata, S.R., Hunt, J.*, Cook, E.C., Creamer, T.P., **Fitzkee N.C.** (2017) "¹H, ¹⁵N, and ¹³C Chemical Shift Assignments of the Regulatory Domain of Human Calcineurin." *Biomolecular NMR Assignments*. 11 (2): 215-219. <https://doi.org/10.1007/s12104-017-9751-x>
 25. Woods, K. E., Perera, Y. R., Davidson, M. B.*, Wilks, C. A.*, Yadav, D. K., **Fitzkee, N. C.** (2016) "Understanding Protein Structure Deformation on the Surface of Gold Nanoparticles of Varying Size." *Journal of Physical Chemistry C*. 120 (49): 27944-27953. <https://doi.org/10.1021/acs.jpcc.6b08089>
 26. Wang, A. Perera, Y.R., Davidson, M.B.*, **Fitzkee, N.C.** (2016) "Electrostatic Interactions and Protein Competition Reveal a Dynamic Surface in Gold Nanoparticle-Protein Adsorption." *Journal of Physical Chemistry C*. 120 (42): 24231-24239. <https://doi.org/10.1021/acs.jpcc.6b08469>
 27. Brown, L.R., Gunnell, S.M., Cassella, A., Keller, L.E., Scherkenbach, L.A. Mann, B., Brown, M.W. Hill, R., **Fitzkee, N.C.**, Rosch, J.W., Tuomanen, E., Thornton, J.A. (2016) "AdcAll of *Streptococcus pneumoniae* affects pneumococcal invasiveness." *PLOS One*. 11 (1): e0146785. <https://doi.org/10.1371/journal.pone.0146785>
 28. Nettles, W., Song, H., Farquar, E., **Fitzkee, N. C.**, Emerson, J. P. (2015) "Characterization of the Copper(II) Binding Sites in Human Carbonic Anhydrase II." *Inorganic Chemistry*. 54 (12): 5671-5680. <https://doi.org/10.1021/acs.inorgchem.5b00057>
 29. Wilder, H., Wozniak, E., Huddleston, E. C., Tata, S., **Fitzkee, N. C.**, and Lopez, J. (2015) "Case Report: A Retrospective Serological Analysis Indicating Human Exposure to Tick-Borne Relapsing Fever Spirochetes in Texas." *PLoS Neglected Tropical Diseases*. 9 (4): e0003617. <https://doi.org/10.1371/journal.pntd.0007215>
 30. Siriwardana, K., Wang, A., Gadogbe, M., Collier, W. E., **Fitzkee, N. C.**, Zhang, D. (2015) "Studying the Effects of Cysteine Residues on Protein Interactions with Silver Nanoparticles." *Journal of Physical Chemistry C*. 119 (5): 2910-16. <https://doi.org/10.1021/jp512440z>

**PUBLICATIONS:
(CONT.)**

31. Wang, A., Vo, T.,* Le, V., **Fitzkee, N. C.** (2014) "Using Hydrogen-Deuterium Exchange to Monitor Protein Structure in the Presence of Gold Nanoparticles." *Journal of Physical Chemistry B*. 118(49): 14148-56. <https://doi.org/10.1021/jp506506p>
32. Wang, A., Vangala, K. Vo, T.,* Zhang, D., **Fitzkee, N. C.** (2014) "A Three-Step Model for Protein-Gold Nanoparticle Adsorption." *Journal of Physical Chemistry C*. **138**: 8134-8142. <https://doi.org/10.1021/jp411543y>
33. Siriwardana K., Wang A., Vangala K., **Fitzkee N. C.**, Zhang D. (2013) "Probing the Effects of Cysteine Residues on Protein Adsorption onto Gold Nanoparticles Using Wild-Type and Mutated GB3 Proteins." *Langmuir*. **29**: 10990-10996. <https://doi.org/10.1021/la402239h>
34. Sgourakis, N. G., Lange, O. F., DiMaio, F., Andre, I., **Fitzkee, N. C.**, Rossi, P., Montelione, G. T., Bax, A., Baker, D. (2011) "Determination of the structures of symmetric homodimers from NMR chemical shifts and residual dipolar couplings." *Journal of the American Chemical Society*. **133**: 6288-6298. <https://doi.org/10.1021/ja111318m>
35. **Fitzkee, N. C.**, Torchia, D.A., Bax, A. (2011) "Measuring rapid hydrogen exchange in the 36 kDa HIV-1 integrase catalytic core domain." *Protein Science*. **20**: 500-512. *Featured on the cover.* <https://doi.org/10.1002/pro.582>
36. **Fitzkee, N. C.**, Bax, A. (2010) "Facile measurement of ¹H-¹⁵N residual dipolar couplings in larger perdeuterated proteins." *Journal of Biomolecular NMR*. **48**: 65-70. <https://doi.org/10.1007/s10858-010-9441-9>
37. **Fitzkee, N. C.**, Masse, J. E., Shen, Y., Davies, D. R., Bax, A. (2010) "Solution conformation and dynamics of the HIV-1 Integrase Core Domain." *Journal of Biological Chemistry*. **285**: 18072-18084. <https://doi.org/10.1074/jbc.M110.11340>
38. **Fitzkee, N. C.**, and García-Moreno E., B. (2008) "Electrostatic interactions in unfolded proteins." *Protein Science*. **17**: 216-227. <https://doi.org/10.1110/ps.073081708>
39. Street, T. O., **Fitzkee, N. C.**, Perskie, L. L., Rose, G. D. (2007) "Physical-chemical determinants of turn conformations in globular proteins." *Protein Science* **16**: 1720-1727. <https://doi.org/10.1110/ps.072898507>
40. **Fitzkee, N. C.**, Rose G. D. (2005) "Sterics and solvation winnow accessible conformational space for unfolded proteins." *Journal of Molecular Biology* **353**: 873-877. *Featured on the cover.* <https://doi.org/10.1016/j.jmb.2005.08.062>
41. **Fitzkee, N. C.**, Fleming P. J., Gong H., Panasik N. Jr., Street T. O., Rose G. D. (2005) "Are proteins made from a limited parts list?" *Trends in Biochemical Sciences* **30**: 73-80. <https://doi.org/10.1016/j.tibs.2004.12.005>
42. **Fitzkee, N. C.**, Fleming, P. J., Rose, G. D. (2005) "The Protein Coil Library: a structural database of non-helix, non-strand fragments derived

**PUBLICATIONS:
(CONT.)**

from the PDB.” *Proteins: Structure, Function, and Bioinformatics* **58**: 852-854. <https://doi.org/10.1002/prot.20394>

43. Fleming P. J., **Fitzkee N. C.**, Mezei M., Srinivasan R., Rose G. D. (2005) “A novel method reveals that solvent water favors polyproline II over beta-strand conformation in peptides and unfolded proteins: conditional hydrophobic accessible surface area (CHASA).” *Protein Science* **14**: 111-118. <https://doi.org/10.1110/ps.041047005>
44. **Fitzkee, N. C.**, Rose, G. D. (2004) “Reassessing random-coil statistics in unfolded proteins.” *Proceedings of the National Academy of Sciences USA* **101**: 12497-12502. <https://doi.org/10.1073/pnas.0404236101>
45. **Fitzkee, N. C.**, Rose, G. D. (2004) “Steric restrictions in protein folding: an alpha-helix cannot be followed by a contiguous beta-strand.” *Protein Science* **13**: 633-639. *Featured on the cover.* <https://doi.org/10.1110/ps.03503304>

**OTHER
PUBLICATIONS:**

Articles published in popular media.

1. **Fitzkee, N.C.** “How Scientists are Fighting Infection-Causing Biofilms” (2018) *The Conversation*. <https://theconversation.com/how-scientists-are-fighting-infection-causing-biofilms-102698>

**INVITED
TALKS:**

1. "Protein Structure and Stability on Surfaces: Form Biomolecular Coronas to Biofilms." (November 2022) Clemson University Chemistry Departmental Seminar Series. Clemson, SC.
2. "Protein Stability on Nanoparticle Surfaces: A Material Difference." (August 2022) 2022 Colorado Protein Stability Conference. Breckenridge, CO.
3. "Using NMR to understand Protein Binding and Structure on Nanoparticle Surfaces." (November, 2021) 2021 Southeast Regional Meeting of the American Chemical Society (SERMACS). Birmingham, AL.
4. "How Proteins Interact with Surfaces and Why You Should Care." (September, 2021) The 35th Gibbs Conference on Biological Thermodynamics. Carbondale, IL.
5. "NMR-based approaches for monitoring protein binding and structure on nanoparticle surfaces." (August, 2021) 261st ACS National Meeting and Exposition. Atlanta, GA.
6. "Challenges and Opportunities during and post COVID-19." (September, 2020) 5th Vanderbilt Gateway NMR Conference. Nashville, TN.
7. "Studying Protein Behavior on Surfaces: From Nanoparticles to Biofilms." (April, 2020) University of Alabama. Tuscaloosa, AL.
8. "How staphylococcal autolysin interacts with surfaces during biofilm formation" (March, 2020) Spring 2020 American Chemical Society National Meeting and Exposition. Philadelphia, PA.
9. "Protein Behavior on Surfaces: From Nanoparticles to Biofilms"(January, 2020) University of Iowa Department of Chemistry. Iowa City, IA.
10. "Understanding the Mechanism of Phase Separation in Elastin-Like Polypeptides." (July, 2019) The 74th Calorimetry Conference. Santa Fe, NM.
11. "Using Histone H1 Derived Peptides to Investigate Binding Affinity and Inter-Domain Dynamics in Human Pin1." (February, 2019) The 63rd Annual Meeting of the Biophysical Society. Baltimore, MD.
12. "Using Nanoparticle-Protein Interactions to Understand Bacterial Biofilm Formation." (February 2019) Department of Bioscience Research, University of Tennessee Health Sciences Center. Memphis, TN.
13. "Structure and Function of Proteins on Nanoparticle Surfaces. (January, 2019) Department of Chemistry, University of Illinois at Urbana-Champaign.
14. "Understanding Protein Structure and Orientation on Gold Nanoparticle Surfaces." (March, 2018) Indian Institute of Technology, Delhi. New Delhi, India.
15. "Structure and Orientation of Proteins on Nanoparticle Surfaces." (February, 2018) University of Southern Mississippi. Department of Chemistry and Biochemistry's Spring 2018 "Graduate Student Choice" seminar.
16. "Understanding Protein Behavior on Gold Nanoparticle Surfaces." (January, 2018) University of West Florida. Pensacola, FL.
17. "Understanding Protein Behavior on Gold Nanoparticle Surfaces." (October, 2017) University of South Alabama. Mobile, AL.
18. "Using Experiment and Simulation to Understand Self-Association in Disordered Elastin-Like Proteins. (September, 2017) US Army Engineer Research and Development Center. Vicksburg, MS.

**INVITED
TALKS:
(CONT.)**

19. "Research in the Fitzkee Lab: Disordered Proteins, Nanoparticles, and Structure." 10th Meeting of the Mississippi Regional Biophysical Consortium. (May, 2017)
20. "Developing a Molecular Understanding of Gold Nanoparticle-Protein Interactions." (October, 2016) University of Iowa Carter College of Medicine. Iowa City, IA
21. "Using Molecular Biophysics to Solve Interesting Problems in Chemistry: The Case of Protein-Surface Interactions." (October, 2016) Samford University. Birmingham, AL.
22. "Developing a Molecular Understanding of Gold Nanoparticle-Protein Interactions." (September, 2016) Iowa State University, Ames, IA.
23. "Developing a Molecular Understanding of Gold Nanoparticle-Protein Interactions." (September, 2016) University of Memphis, Memphis, TN.
24. "Scratching the Surface of the Nanoparticle Interface: The Physical Principles Behind Protein Adsorption." (September, 2016) Mississippi State University, Starkville, MS.
25. "Developing a Molecular Understanding of Gold Nanoparticle-Protein Interactions." (September, 2016) Jackson State University, Jackson, MS.
26. "Developing a Molecular Understanding of Gold Nanoparticle-Protein Interactions." (August, 2016) University of Alabama, Tuscaloosa, AL.
27. "Electrostatic Interactions at the Protein-Nanoparticle Interface." (June, 2016) The Bax Symposium. Bethesda, MD.
28. "Simulations of Unfolded Proteins: Seeing is Deceiving." (May, 2016) The Ninth Annual Meeting of the Mississippi Regional Biophysical Consortium. Starkville, MS.
29. "Developing a Molecular Understanding of Gold Nanoparticle-Protein Interactions." (April 2016) Brown University, Providence RI.
30. "How Do Nanoparticle Size and Protein Charge Affect Gold Nanoparticle-Protein Interactions?" (March, 2016) The 60th Annual Meeting of the Biophysical Society. Los Angeles, CA.
31. "Using NMR Spectroscopy to Understand the Thermodynamics of Gold Nanoparticle-Protein Interactions." (November, 2015) The 2015 Combined Southeast-Southwest Meeting of the American Chemical Society. Memphis, TN.
32. "Using NMR to Monitor Protein Structure on Nanoparticle Surfaces." (February, 2015) The 2016 Meeting of the Mississippi Academy of Sciences. Hattiesburg, MS.
33. "Protein Folding in Adverse Conditions: Nanoparticle Surfaces and Non-Native States." (March, 2014) Southeastern Louisiana University, Department of Chemistry. Hammond, LA.
34. "Protein Folding in Adverse Conditions: Nanoparticle Surfaces and Non-Native States." (May, 2014) University of Kentucky, Department of Structural Biology. Louisville, KY.
35. "Unraveling the Unfolded State: Exploring the Limitations of Experimental Data" (September, 2014) Mississippi State University Department of Chemistry. Starkville, MS.

**INVITED
TALKS:
(CONT.)**

36. Protein Folding in Adverse Conditions: Nanoparticle Surfaces and Non-Native States.” (November, 2014) Mississippi State University College of Veterinary Medicine. Starkville, MS.
37. “An NMR-based model for protein-gold nanoparticle interactions.” (November, 2013) 2013 Southeast Regional Meeting of the ACS. Atlanta, GA.
38. “Studying the folding of individual residues in a small protein.” (October, 2013) 27th Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
39. “Biophysical studies of protein-nanoparticle interactions.” (May, 2013) 6th Annual Meeting of the Mississippi Regional Biophysics Consortium. Starkville, MS.
40. “NMR studies for understanding disordered protein states.” (April, 2013) University of Alabama at Birmingham. Birmingham, AL.
41. “Adventures in disordered proteins: From denatured states to nanoparticles.” (March, 2013) Texas State University at San Martin. San Martin, TX.
42. “An NMR-derived model for protein-nanoparticle adsorption.” (February, 2013) 77th Annual Meeting of the Mississippi Academy of Sciences. Hattiesburg, MS.
43. “Adventures in disordered proteins: From denatured states to nanoparticles.” (October, 2012) University of Alabama at Huntsville. Huntsville, AL.
44. “NIH Career Symposium 2012 – Academic Jobs Panel.” (May, 2012) National Institutes of Health. Bethesda, MD.
45. “Dynamics and Function in the Catalytic Domain of HIV Integrase.” (September, 2011) University of North Alabama. Florence, AL.
46. “Structure and Dynamics of Large Protein Systems: Progress with HIV-1 Integrase.” (June, 2011) 4th Mississippi State Biophysical Consortium. Oxford, MS.
47. “Solution NMR of HIV-1 integrase: Toward an understanding of the full length enzyme.” (August, 2010) XXIVth International Conference on Magnetic Resonance in Biological Systems. Cairns, Australia.
48. “Electrostatic properties of the unfolded state: What can we learn from modeling?” (August, 2007) The 234th National Meeting of the American Chemical Society. Boston, MA.
49. “Modeling electrostatic properties of unfolded *Staphylococcal* nuclease.” (March, 2007) The Fifty-First Annual Meeting of the Biophysical Society. Baltimore, MD.
50. “Electrostatic effects in the unfolded state of *Staphylococcal* nuclease.” (November, 2006) The Institute for Multiscale Modeling of Biological Interactions Second Annual Retreat. Baltimore, MD.
51. “Conformational principles for organizing the denatured state.” (February, 2006) The Fiftieth Annual Meeting of the Biophysical Society. Salt Lake City, UT.
52. “How sterics and solvation reduce the size of protein conformational space.” (October, 2005) The Nineteenth Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.

53. "Conditional hydrophobic accessible surface area: A novel method of calculating solvation energies in proteins." (November, 2004) The First Annual Biological Language Conference. Pittsburgh, PA.

**STUDENT
POSTERS/
TALKS:**

Contributed poster presentations/talks with students since 2011. Presenting authors are italicized. Undergraduate contributors are noted with an asterisk. Student abstracts selected for an oral presentation and travel awards are indicated explicitly.

1. *Wilson, C., Ibrahim, A.Y., Correia, J.J., **Fitzkee, N.C.**, Lewis, K.A., Hough, L.E., Whitten, S.T. (2022) "ParSe Version 2: A Second-Generation Predictor of Protein Phase Separation based upon Intrinsic Sequence-based Properties."* 36th Annual Gibbs Conference on Biological Thermodynamics. Carbondale, IL.
2. *Shaikh, T., **Fitzkee, N.C.** (2022) "In Situ Tracking of Serum Albumin Binding to Gold Nanoparticles in the Presence of Serum and Serum Proteins."* 36th Annual Gibbs Conference on Biological Thermodynamics. Carbondale, IL.
3. *Amarasekara, D., Kariyawasam, C.S., Hejny, M.,* **Fitzkee, N.C.** (2022) "Using Protein Engineering to Improve Thermal Response in Anti-Biofilm Gold Nanoparticles."* 36th Annual Gibbs Conference on Biological Thermodynamics. Carbondale, IL.
4. *Kariyawasam, C.S., Somarathne, R.P., Mayatt, R.S.,* Conner, R.A.,* **Fitzkee, N.C.** (2022) "Protein Charge Distribution Influences the Nature of the Nanoparticle Protein Corona."* 36th Annual Gibbs Conference on Biological Thermodynamics. Carbondale, IL.
5. *Somarathne, R.P., Amarasekara, D., Kariyawasam, C.S., Robertson, H.,* **Fitzkee, N.C.** (2022) "Protein destabilization and unfolding on polystyrene nanoparticles of varying size."* 36th Annual Gibbs Conference on Biological Thermodynamics. Carbondale, IL.
6. *Kariyawasam, C.S., Somarathne, R.P., Mayatt, R.S.,* Conner, R.A.,* **Fitzkee, N.C.** (2022) "Protein Charge Distribution Influences the Nature of the Nanoparticle Protein Corona."* 2022 Colorado Protein Stability Conference. Breckenridge, CO.
7. *Somarathne, R.P., Amarasekara, D., Kariyawasam, C.S., Robertson, H.,* **Fitzkee, N.C.** (2022) "Protein destabilization and unfolding on polystyrene nanoparticles of varying size."* 2022 Colorado Protein Stability Conference. Breckenridge, CO.
8. *Zhu, X.X., Alom, M.S., Yadav, R., **Fitzkee, N.C.** (2022) "Predicting Protein Function and Orientation on a Gold Nanoparticle Surface Using a Residue-Based Affinity Scale."* Experimental Biology 2022. Philadelphia, PA.
9. *Yadav, R., Shen, Y., Somarathne, R.P., McConnell, K.D., Park, J.Y., **Fitzkee, N.C.** (2022) "NMR Illuminates Ligand and Surface Adsorption of Autolysin-Amidase from *Staphylococcus epidermidis*."* The 66th Annual Meeting of the Biophysical Society, San Francisco, CA.
10. *Somarathne, R.P., Chappell, E.R.,* Perera, Y.R., Yadav, R., Park, J.Y., **Fitzkee, N.C.** (2021) "Staphylococcal autolysin domains bind polystyrene surfaces and can impede biofilm formation."* 2021 Southeast Regional Meeting of the American Chemical Society (SERMACS). Birmingham, AL.
11. *Yadav, R., Shen, Y., McConnell, K.D., Somarathne, R.P., **Fitzkee, N.C.** (2021) "Insights into the Surface Adsorption and Structure-Function Characterization of Autolysin-Amidase from *S. epidermidis*."* 261st Southeast Regional Meeting of the American Chemical Society (SERMACS). Birmingham, AL.
12. *Amarasekara, D.L., Kariyawasam, C.S., Hejny, M.A.,* **Fitzkee, N.C.** (2021) "Engineering Thermo-Responsive Gold Nanoparticles for Photothermal Therapy."* Southeast Regional Meeting of the American Chemical Society (SERMACS). Birmingham, AL.

13. Somarathne, R.P., Chappell, E.R.,* Perera, Y.R., Yadav, R., Park, J.Y., **Fitzkee, N.C.** (2021) "Staphylococcal autolysin domains bind polystyrene surfaces and can impede biofilm formation." The 35th Annual Gibbs Conference on Biological Thermodynamics. Carbondale, IL.
14. Yadav, R., Shen, Y., McConnell, K.D., Somarathne, R.P., **Fitzkee, N.C.** (2021) "Insights into the Surface Adsorption and Structure-Function Characterization of Autolysin-Amidase from *S. epidermidis*." The 35th Annual Gibbs Conference on Biological Thermodynamics. Carbondale, IL.
15. Amarasekara, D.L., Kariyawasam, C.S., Hejny, M.A.,* **Fitzkee, N.C.** (2021) "Engineering Thermo-Responsive Gold Nanoparticles for Photothermal Therapy." The 35th Annual Gibbs Conference on Biological Thermodynamics. Carbondale, IL.
16. Somarathne, R.P., Chappell, E.R.,* Perera, Y.R., Yadav, R., Park, J.Y., **Fitzkee, N.C.** (2021) "Staphylococcal autolysin domains bind polystyrene surfaces and can impede biofilm formation." 261st ACS National Meeting and Exposition. Atlanta, GA. Oral presentation.
17. Yadav, R., Shen, Y., McConnell, K.D., Somarathne, R.P., **Fitzkee, N.C.** (2021) "Insights into the Surface Adsorption and Structure-Function Characterization of Autolysin-Amidase from *S. epidermidis*." 261st ACS National Meeting and Exposition. Atlanta, GA. Oral presentation.
18. Amarasekara, D.L., Kariyawasam, C.S., Hejny, M.A.,* **Fitzkee, N.C.** (2021) "Engineering Thermo-Responsive Gold Nanoparticles for Photothermal Therapy." 261st ACS National Meeting and Exposition. Atlanta, GA.
19. Yadav, R., **Fitzkee, N.C.** (2020) "Structural Characterization and Surface Adsorption of *S. epidermidis* Autolysin E-Amidase a Protein Implicated in Biofilm Formation". The 64th Annual Meeting of the Biophysical Society, San Diego, CA. Oral presentation.
20. Hill, R.A., Claxton, S.E.,* Boulet, K.J.,* Perera, Y.R., South, T.M.,* Yadav, R., and **Fitzkee, N.C.** (2020) "Investigating Thermodynamics and Kinetic Control Mechanism for Competitive Protein Adsorption to a Nanoparticle Surface." 259th ACS National Meeting, Philadelphia, PA. Selected for Oral Presentation.
21. McConnell, K.D., Williams, O.C., * Chappell, E.R., * Manns, R.G., * **Fitzkee, N.C.** (2020) "Spectroscopic Investigation of Gold Nanoparticle-Protein Interactions." The 259th ACS National Meeting. Philadelphia, PA.
22. Chappell, E.R.,* Somarathne, R.D., Perera, Y.R., **Fitzkee, N.C.** (2020) "Interactions of R2ab and Amidase with Polystyrene Nanoparticles." 2020 Shackouls Honors College Fall Undergraduate Research Symposium. Starkville, MS.
23. Chappell, E.R.,* Somarathne, R.D., Perera, Y.R., **Fitzkee, N.C.** (2020) "Interactions of R2ab and Amidase with Polystyrene Nanoparticles." The 2020 NSF REU: Food, Energy, and Water Security Symposium. Starkville, MS.
24. Perera, Y.R., South, T.M., McConnel, K.D., Yadav, R., * **Fitzkee, N.C.** (2020) "Structure-Function Relationship in Biofilms Characterizing the Staphylococcal Autolysin R2 Repeat Domain." The 64th Annual Meeting of the Biophysical Society. San Diego, CA. Selected for Oral Presentation.
25. Alom, M.S., Jackson, S.*, Perera, Y.R., Yadav, R., **Fitzkee, N.C.** (2020) "A Host-Guest System for Understanding Protein-Nanoparticle Interactions." The 64th Annual Meeting of the Biophysical Society. San Diego, CA.

**STUDENT
POSTERS/
TALKS:
(CONT.)**

26. *Hill, R.A., Boulet, K.J.,* Claxton, S.E.,* Pererea, Y.R., South, T.M.,* Fitzkee, N.C.* (2019) "Investigating Competitive Protein Adsorption to a Nanoparticle Surface." The 33rd Annual Gibbs Conference on Biothermodynamics. Carbondale, IL. Selected for Oral Presentation.
27. *Fitzkee, N.C., McConnell, K.D., Williams, O.W.*, Chappell, E.R.,* Manns, R.G.** (2019) "Thermodynamics of Protein-Surface Binding: The Model Makes all the Difference." The 33rd Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
28. *Alom, M.S., Jackson, S.,* Perera, Y.R., Fitzkee, N.C.* (2019) "Predicting of Protein Adsorption to Nanoparticle Surfaces: A Competition Approach." The 33rd Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
29. *South, T.M.,* Perera, Y.R., Yadav, R. Hill, R.A., Fitzkee, N.C.* (2019) "NMR Assignment and Surface Binding Characterization of R2ab, A Staphylococcal Protein Involved in Biofilms." The 33rd Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
30. *McConnell, K.D., Williams, O.W.*, Fitzkee, N.C.* (2019) "Combined Calorimetric and Spectroscopic Approaches to Investigate Gold Nanoparticle-Protein Interactions." (2019) The 74th Calorimetry Conference. Santa Fe, NM. Selected for Oral Presentation.
31. *Chappell, E.R.,* McConnell, K.D., Williams, O.W.,* Manns, R.D.,* Fitzkee, N.C.* (2019) "Thermodynamics of Protein Binding to Gold Nanoparticles Monitored by Synchronous Fluorescence Spectroscopy and Dynamic Light Scattering." (2019) The 74th Calorimetry Conference. Santa Fe, NM.
32. *Jackson, S.,* Alom, M.S., Perera, Y.R., Fitzkee, N.C.* (2019) "Introducing Mutations in the GB3 Protein to Understand Gold Nanoparticle Interactions." The 2019 Mississippi IDeA Conference. Jackson, MS. First place poster award winner.
33. *Strickert, K.,* Williams, R.B., Fitzkee, N.C.* (2019) "Does Binding to a Nanoparticle Change a Protein's Structure?" MSU 2019 Summer Undergraduate Research Symposium. Starkville, MS.
34. *Manns, R.D.,* McConnell, K.D., Williams, O.W.*, Chappell, E.R.,* Fitzkee, N.C.* (2019) "Thermodynamics of Protein Binding to Gold Nanoparticles Monitored by Synchronous Fluorescence Spectroscopy and Dynamic Light Scattering." MSU 2019 Summer Undergraduate Research Symposium. Starkville, MS.
35. *Williams, O.*, McConnell, K., Fitzkee N.C.* (2019) "Understanding the thermodynamics of protein-surface interactions using 15 nm gold nanoparticles." MSU 2019 Spring Undergraduate Research Symposium. Starkville, MS.
36. *Claxton, S.E.,* Hill, R.E., Boulet, K.J.,* Fitzkee, N.C.* (2019) "Quantification of AuNP-Protein Interactions via NMR." MSU 2019 Spring Undergraduate Research Symposium. Starkville, MS.
37. *Hill, R.A., Boulet, K.J.*, Perera, Y.R., Davidson, M.B., Fitzkee, N.C.* (2019) "Investigating How Protein Mixtures Interact with Gold Nanoparticles." The 63rd Annual Meeting of the Biophysical Society. Baltimore, MD.
38. *Perera, Y.R., Hughes, A., Fitzkee, N.C.* (2019) "The Adsorption Kinetics of Biomolecules on to PEGylated Gold Nanoparticles." The 63rd Annual Meeting of the Biophysical Society. Baltimore, MD. *BPS Travel Award Winner.*

**STUDENT
POSTERS/
TALKS:
(CONT.)**

39. *Jinasena D.*, Bowleg, J., Simmons, R.H.*, Zhang, Y., Gwaltney S.R., **Fitzkee N.C.** (2018) "Understanding how Pin1 Substrate Interactions Modulate Affinity and Inter-Domain Dynamics." The 32nd Annual Gibbs Conference on Biothermodynamcs. Carbondale, IL. Oral Presentation.
40. *Davidson M.B.*, Perera Y.R., South T.M.*, **Fitzkee N.C.** (2018) "Understanding How the R2ab Domain from Staphylococcal Autolysin E Interacts with Nanoparticle Surfaces." The 32nd Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
41. *Perera Y.R.*, Hughes A.*, **Fitzkee N.C.** (2018) "Does PEGylation Inhibit Protein Binding to Gold Nanoparticles?" The 32nd Annual Gibbs Conference on Biothermodynamcs. Carbondale, IL.
42. *Boulet, K.J.**, Hill, R.A., Perera, Y.R., **Fitzkee, N.C.** (2018) "Using Two-Dimensional NMR to Understand How Protein Mixtures Interact with Gold Nanoparticles." The 2018 MSU Summer Undergraduate Research Symposium. Starkville, MS.
43. **Fitzkee, N.C.**, Perera, Y.R. (2018) "NMR Spectroscopy: A Useful Tool for Studying Proteins on Gold Nanoparticle Surfaces." 2018 Noble Metal Nanoparticles Gordon Research Conference. Mount Holyoke College, South Hadley, MA.
44. *Perera, Y.R.*, Hughes, A.*, **Fitzkee, N.C.** (2018) "The Adsorption Kinetics of Biomolecules on to PEGylated Gold Nanoparticles." 2018 Noble Metal Nanoparticles Gordon Research Conference. Mount Holyoke College, South Hadley, MA.
45. *Perera, Y.R.*, Hughes, A.*, **Fitzkee, N.C.** (2018) "Structure and Orientation of a Small Protein on a Gold Nanoparticle Surface." The 255th American Chemical Society National Meeting & Exposition. New Orleans, LA. Oral Presentation.
46. *Jinasena, D.*, Gyamfi, H., **Fitzkee, N.C.** (2018) "Pin1-Histone H1 Interactions: Towards an understanding of Substrate Specific Activity. The 255th American Chemical Society National Meeting & Exposition. New Orleans, LA.
47. *Hill, R.A.* Byers, A.H.*, Hunt, J.J.*, Sanders, E.*, Mlsna, T.E., **Fitzkee, N.C.** (2018) "An NMR Based Metabolomics Approach to Understanding Biochar's Effects on *Escherichia coli*." The 255th American Chemical Society National Meeting & Exposition. New Orleans, LA.
48. **Fitzkee, N.C.**, Perera, Y.R. (2018) "Structure and Orientation of a Small Protein on a Gold Nanoparticle Surface" The 62nd Annual Meeting of the Biophysical Society. San Francisco, CA.
49. *Sanders, E.**, Hill, R.A., Hunt, J.J.*, Mlsna, T.E., **Fitzkee, N.C.** (2017) Understanding Biochar's Effects on Bacterial Metabolites using Quantitative NMR Techniques. The 2017 MSU Summer Undergraduate Research Symposium. Starkville, MS.
50. *Jinasena, J.*, Gyamfi, H., **Fitzkee, N.C.** (2017) "An NMR Study of Pin1-Histone H1 Interactions." The 2017 Southeast Meeting of the American Chemical Society. Charlotte, NC. Oral presentation.
51. *Zhang, Y.*, Price, C.J.*, Pratt, G.L.*, Bidwell, G.L. Correia, J.J., **Fitzkee, N.C.** (2017) "Observation of Intermolecular Interactions and Dynamics in the Early Stages of ELP Phase Separation." The Thirty-First Annual Gibbs Conference on Biothermodynamcs. Carbondale, IL. Oral presentation.

**STUDENT
POSTERS/
TALKS:
(CONT.)**

52. *Jinasena, J., Gyamfi, H., Fitzkee, N.C.* (2017) "An NMR Study of Pin1-Histone H1 Interactions." The Thirty-First Annual Gibbs Conference on Biothermodynamcs. Carbondale, IL.
53. *Perera, Y.R., Hughes, A.*, Fitzkee, N.C.* (2017) "Structure and Orientation of a Small Protein on a Gold Nanoparticle Surface." The Thirty-First Annual Gibbs Conference on Biothermodynamcs. Carbondale, IL.
54. *Zhang, Y., Price, C.J.*, Pratt, G.L.*, Bidwell, G.L. Correia, J.J., Fitzkee, N.C.* (2017) "Modeling the Early Stages of Aggregation in Disordered Elastin-Like Proteins." The 60th Annual Meeting of the Biophysical Society. New Orleans, LA. Oral presentation.
55. *Ezzell, N.*, Zhang, Y., Whitten, S. T., Fitzkee, N. C.* (2017) "Improving the Performance of Simulations of the Intrinsically Disordered N-Terminal Domain from p53." The 60th Annual Meeting of the Biophysical Society. New Orleans, LA.
56. *Hunt, J.J.*, Yadav, D.K., Cook, E., Creamer, T., Fitzkee, N.C.* (2017) "Chemical Shift Assignment of the Regulatory Domain of Calcineurin with NMR Spectroscopy." The 60th Annual Meeting of the Biophysical Society. New Orleans, LA.
57. *Zhang, Y., Price, C. J.*, Pratt, G. L.*, Bidwell, G. L., Correia, J. J., Fitzkee, N. C.* (2016) "Investigating the Intermolecular Interactions in the Early Stages of ELP Aggregation." The Thirtieth Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
58. *Perera, Y. R., Wang, A., Hughes, A.*, Fitzkee, N. C.* (2016) "Modulating Protein-Nanoparticle Interaction Energetics Using Site-Directed Mutagenesis." The Thirtieth Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
59. *Price, C. J.*, Pratt, G. L.*, Zhang, Y., Fitzkee, N. C.* (2016) "Elucidating Structure in the Early Stages of Aggregation in Elastin-Like Proteins." The 2016 MSU Summer Undergraduate Research Symposium. Starkville, MS.
60. *Perera, Y.R., Hughes, A. C.*, Perera, R., Wang, A., Fitzkee, N. C.* (2016) "Modulating Protein-Nanoparticle Binding Capacity Using Site-Directed Mutagenesis" The Ninth Annual Meeting of the Mississippi Regional Biophysical Consortium. Starkville, MS. *Oral Presentation.*
61. *Ezzell, N.*, Zhang, Y., Fitzkee, N.C.* (2016) "Modeling Intrinsically Disordered Proteins with Chemically Realistic Monte-Carlo Simulations." The Ninth Annual Meeting of the Mississippi Regional Biophysical Consortium. Starkville, MS.
62. *Price, C. J.*, Zhang, Y., Fitzkee, N.C.* (2016) "Synthesis of MTSL-Labeled Elastin-Like Proteins for Paramagnetic NMR and EPR." The Ninth Annual Meeting of the Mississippi Regional Biophysical Consortium. Starkville, MS.
63. *Zhang, Y., Price, C. J.*, Fitzkee, N.C.* (2016) "Studying ELP Aggregation Using Paramagnetic Methods." The Ninth Annual Meeting of the Mississippi Regional Biophysical Consortium. Starkville, MS.
64. *Hughes, A. C.*, Perera, R., Wang, A., Fitzkee, N. C.* (2016) "Using Site-Directed Mutagenesis to Investigate Protein-Nanoparticle Adsorption" The 2016 MSU Spring Undergraduate Research Symposium, Mississippi State, MS.

- STUDENT POSTERS/TALKS: (CONT.)**
65. *Tran, M. T.,* Hill, R., Fitzkee, N.C.* (2016) "Examining Bacterial Metabolite Concentrations using NMR Spectroscopy" The 2016 MSU Spring Undergraduate Research Symposium, Mississippi State, MS.
 66. *Hunt, J.J.,* Yadav, D.K., Fitzkee, N.C.* (2016) "Purification and Isotopic Labeling of the Regulatory Domain of Calcineurin" The 2016 MSU Spring Undergraduate Research Symposium, Mississippi State, MS.
 67. *Price, C. J.,* Zhang, Y., Fitzkee, N.C.* (April 2016) "Synthesis of MTSL-Labeled Elastin-Like Proteins for Paramagnetic NMR and EPR" Mississippi State University's Summer Undergraduate Research Symposium. *Oral presentation.*
 68. *Ezzell, A. N.,* Zhang, Y., Fitzkee, N.C.* (2016) "Modeling Intrinsically Disordered Proteins with Chemically Realistic Monte-Carlo Simulations" The 2016 MSU Spring Undergraduate Research Symposium, Mississippi State, MS. *Third place poster award.*
 69. *Price, C. J.,* Zhang, Y., Fitzkee, N.C.* (2015) "Synthesis of MTSL-Labeled Elastin-Like Proteins for Paramagnetic NMR" The 2015 Combined Southeast-Southwest Meeting of the American Chemical Society, Memphis, TN.
 70. *Jinasena, D.S., Gyamfi, H., and Fitzkee, N.C.* (2015) "Exploring the Thermodynamics of the Pin1-Histone H1 Interaction." The 2015 Combined Southeast-Southwest Meeting of the American Chemical Society. Memphis, TN. Oral presentation.
 71. *Perera, Y.R., Woods, K.E., Wang, A., and Fitzkee, N.C.* (2015) "Chemical Methylation of Lysine residues Can Severely Weaken Gold Nanoparticle-Protein Interactions." The 2015 Combined Southeast-Southwest Meeting of the American Chemical Society. Memphis, TN. Oral presentation.
 72. *Yadav, D.K., Tata, S.R. Cook, E.C., Creamer, T.P., Fitzkee, N.C.* (2015) "NMR Investigation of Calmodulin-Induced Folding in the Regulatory Domain of Calcineurin." The 29th Gibbs Conference on Biothermodynamics. Carbondale, IL.
 73. *Wang, A., Perera, R., Kay, A.,* Hughes, A* and Fitzkee, N. C.* (2015) "Understanding the Electrostatics Contribution to Gold Nanoparticle-Protein Binding." The 29th Gibbs Conference on Biothermodynamics. Carbondale, IL.
 74. *Zhang, Y., Zai-Rose, V., Price, C. J.*, Bidwell, G. L. 3rd., Correia, J. J., and Fitzkee, N. C.* (2015) "Simulating the Early Stages of ELP Aggregation Using a Biased Structural Model." The 29th Gibbs Conference on Biothermodynamics. Carbondale, IL.
 75. *Wilks, C.,* Davidson, M.,* Woods, K., Fitzkee, N.C.* (2015) "How Does Increasing Gold Nanoparticle Size Affect Protein Adsorption?" The Vanderbilt Research Fair. Nashville, TN
 76. *Davidson, M.,* Wilks, C.,* Woods, K., Fitzkee, N.C.* (2015) "How Does Increasing Gold Nanoparticle Size Affect Protein Adsorption?" 2015 Summer Undergraduate Research Conference. Mississippi State, MS.
 77. *Woods, K. E., Wang, A. Kay, A.,* Fitzkee, N. C.* (2015) "Does surface curvature influence protein-nanoparticle interactions?" The 8th Mississippi Regional Biophysics Consortium. Oxford, MS.

- STUDENT POSTERS/TALKS: (CONT.)**
78. *Zhang, Y., Bidwell, G. L., Correia, J. J., Fitzkee, N. C.* (2015) "Studying ELP Aggregation Using Computational Methods and NMR." The 8th Mississippi Regional Biophysics Consortium. Oxford, MS.
 79. *Perera, Y. R., Wang, A., Woods, K. E., Fitzkee, N. C.* (2015) "Modulating Protein-Nanoparticle Interactions using Protein Chemical Modification." The 8th Mississippi Regional Biophysics Consortium. Oxford, MS.
 80. *Madsen, K., *Yadav, D., Fitzkee, N.C.* "Analysis of NMR Data to Investigate Protein Dynamics." The 2016 Meeting of the Mississippi Academy of Sciences. Hattiesburg, MS. Oral presentation.
 81. *Wang, A., Woods, K., Vo, T.,* Coats, D. A.,* Fitzkee, N. C.* (2015) "Monitoring Protein Structure on the Surface of Gold Nanoparticles using NMR Spectroscopy." The 59th Meeting of the Biophysical Society. Baltimore, MD.
 82. *Yadav, D., Fitzkee, N.C.* (2014) "Characterizing the Residue Specific Folding-Unfolding Behavior of a Small Model Protein." The 4th Annual Lester Andrews Graduate Research Symposium. Starkville, MS. Selected for oral presentation.
 83. *Wang, A., Vo, T.,* Le, V., and Fitzkee, N.C.* (2014) "Characterization of Protein-Gold Nanoparticle Interactions by Hydrogen/Deuterium Exchange." The 4th Annual Lester Andrews Graduate Research Symposium. Starkville, MS. Selected for oral presentation.
 84. *Zhang, Y., and Fitzkee, N.C.* (2014) "How unfolded are unfolded proteins? A new strategy to assess unfolded protein NMR measurements." The 4th Annual Lester Andrews Graduate Research Symposium. Starkville, MS. Selected for oral presentation.
 85. *Tata, S.R., Cook, E.C., Creamer, T.P., Fitzkee, N.C.* (2014) "Nuclear Magnetic Resonance Assignments of Calcineurin Regulatory Domain – an Intrinsically Disordered Protein (IDP) and Binding studies with Ca²⁺/Calmodulin (CaM)" The 66th Southeast Regional Meeting of the American Chemical Society (SERMACS). Nashville, TN. Selected for oral presentation.
 86. *Wang, A., Vo, T.,* Le, V., and Fitzkee, N.C.* (2014) "Characterization of Protein-Gold Nanoparticle Interactions by Hydrogen/Deuterium Exchange." The 66th Southeast Regional Meeting of the American Chemical Society (SERMACS). Nashville, TN. Selected for oral presentation.
 87. *Yadav, D.K., Madsen, K* and Fitzkee, N.C.* (2014) "How does the Structure Influence the Folding Pathway in GB3?" The 28th Annual Gibbs Conference on Biothermodynamics. Carbondale, IL. Selected for oral presentation.
 88. *Coats, D. A.,* Woods, K., Wang, A. and Fitzkee, N. C.* (2014) "Understanding How Surface Curvature Modulates Gold Nanoparticle-Protein Interactions" The 2014 Summer Undergraduate Research Conference. Mississippi State, MS.
 89. *Wang, A., Vo, T.,* Le, V., and Fitzkee, N.C.* (2014) "Characterization of protein-gold nanoparticle interactions by hydrogen/deuterium exchange." The XXVIth International Conference on Magnetic Resonance on Biological Systems. Dallas, TX.

**STUDENT
POSTERS/
TALKS:
(CONT.)**

90. *Zhang, Y.*, and **Fitzkee, N.C.** (2014) "How Disordered? Assessing NMR-based Studies of Denatured Proteins." The XXVIth International Conference on Magnetic Resonance on Biological Systems. Dallas, TX.
91. *Yadav, D.K.*, Madsen, K.* and **Fitzkee, N.C.** (2014) "Characterizing the Folding and Unfolding Pathways for a Small Model Protein." The XXVIth International Conference on Magnetic Resonance on Biological Systems. Dallas, TX.
92. *Tata, S. R.*, Maccha, V.R., Lewis, E. A., and **Fitzkee, N.C.** (2014) "Structural Investigation of H1.0 Globular domain on DNA Binding." The XXVIth International Conference on Magnetic Resonance on Biological Systems. Dallas, TX.
93. *Vo, T.*, **Yadav, D.*, **Fitzkee, N. C.** (2014) "Comparing Partially Denatured and Natively Unfolded Protein States." 46th ACS Southeast Undergraduate Research Conference. Knoxville, TN.
94. *Gyamfi, H.*, **Fitzkee, N. C.** (2013) "Understanding binding-induced conformational change in Pin1" 2013 Southeast Regional Meeting of the American Chemical Society. Atlanta, GA.
95. *Zhang, Y.*, **Fitzkee, N. C.** (2013) "How Disordered? Assessing NMR-based studies of denatured proteins." The Twenty-Seventh Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
96. *Yadav, D.*, **Fitzkee, N. C.** (2013) "Characterizing the folding and unfolding pathways for a small model protein." The Twenty-Seventh Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
97. *Wang, A.*, Vangala, K., Zhang, D., **Fitzkee, N. C.** (2013) "Two-Step Model for Protein-Gold Nanoparticle Interactions." The Twenty-Seventh Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
98. *Yadav, D.*, **Fitzkee, N. C.** (2013) "Characterizing the folding and unfolding pathways for a small model protein." The 27th Symposium of the Protein Society. Boston, MA. Selected for a student travel award.
99. *Wang, A.*, **Fitzkee, N. C.** (2013) "Investigation on the interactions between gold nanoparticles and proteins" 3rd Annual Lester Andrews Symposium. Starkville, MS. Student oral presentation.
100. *Wang, A.*, Vangala, K., Zhang, D., **Fitzkee, N. C.** "Characterizing protein-nanoparticle adsorption by NMR." 2013 Keystone Symposium on Frontiers of NMR in Biology. Salt Lake City, UT.
101. *Vo, T.**, Wang, A., Blatt, O., Friedler, A., **Fitzkee, N. C.** (2012) "How does Rev regulate retroviral integration in HIV?" 245th American Chemical Society National Meeting and Exposition. New Orleans, LA.
102. *Wang, A.*, **Fitzkee, N. C.** (2012) "Why do Proteins Bind to Gold Nanoparticles?" The Twenty-Sixth Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
103. *Yadav, D.*, **Fitzkee, N. C.** (2012) "Residue-Specific Unfolding Stabilities and Kinetics in a Small Protein." The Twenty-Sixth Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
104. *Vo, T.**, Wang, A., Blatt, O., Friedler, A., **Fitzkee, N. C.** (2012) "How does Rev regulate retroviral integration in HIV?" MSU 2012 Summer Research Symposium. Starkville, MS.

**STUDENT
POSTERS/
TALKS:
(CONT.)**

105. *Buchanan, W. **, **Fitzkee, N. C.** (2012) "Numerical integration of chemical kinetics equations: A physical chemistry approach for non-programmers." ACS Southeast Undergraduate Research Conference. Starkville, MS.
106. **Fitzkee, N. C.**, Torchia, D. A., Bax, A. (2011) "Measuring rapid hydrogen exchange in large proteins using NMR spectroscopy." The Twenty-Fifth Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
107. **Fitzkee, N. C.**, Masse, J. E., Shen, Y., Davies, D. R., Bax, A. (2010) "Solution conformation of the HIV-1 integrase catalytic core domain: A magnesium-induced structural transition." The Twenty-Fourth Symposium of the Protein Society. San Diego, CA.
108. **Fitzkee, N. C.**, Grishaev, A., Ying, J., Bax, A. (2009) "A combined NMR and small-angle X-ray scattering approach reveals that Pin1's domains bind independent targets." The 2009 NIH Research Festival. Bethesda, MD.
109. **Fitzkee, N. C.**, Grishaev, A., Ying, J., Bax, A. (2009) "Orienting the domains of Pin1 using small angle X-ray scattering and residual dipolar couplings." The Keystone Symposium for Frontiers on NMR in Biology. Santa Fe, NM.
110. **Fitzkee, N. C.**, García-Moreno E., B., Rose, G. D. (2007) "How random are random coils? Quantifying the disorder in the unfolded state." The Twenty-First Symposium of the Protein Society. Boston, MA.
111. **Fitzkee, N. C.**, García-Moreno E., B. (2006) "Modeling electrostatic properties of unfolded *Staphylococcal* nuclease." The Twentieth Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
112. **Fitzkee, N. C.**, Rose, G. D. (2006) "How sterics and solvation reduce the size of protein conformational space." The 2006 Gordon Research Conference on Biopolymers. Newport, RI.
113. **Fitzkee, N. C.**, Rose, G. D. (2004) "The protein denatured state: How organized is it?" The Eighteenth Annual Gibbs Conference on Biothermodynamics. Carbondale, IL.
114. **Fitzkee, N. C.**, Rose, G. D. (2004) "Ramachandran revisited: steric restrictions beyond the dipeptide level." The Forty-Eighth Annual Meeting of the Biophysical Society. Baltimore, MD.