Steffen Lindert

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EDUCATION

2011	PhD in Chemical and Physical Biology (Molecular Biophysics track) Vanderbilt University School of Medicine Advisors: Jens Meiler, Ph.D. and Phoebe Stewart, Ph.D. Dissertation Project: *CryoEM guided de novo protein fold elucidation*
2006	M.S. Physics (1.1, on a scale of 1.0 (best) to 4.0) University of Leipzig, Germany Advisors: Josef Käs, Ph.D. and Herbert Schmiedel, Ph.D. Thesis Project: *Investigation of Nanoparticles in Aqueous Solution with Light Scattering and Small Angle Neutron Scattering*
2002	B.S. Physics (1.3, on a scale of 1.0 (best) to 4.0) University of Leipzig, Germany

RESEARCH POSITIONS AND WORK EXPERIENCE

2021–present	Associate Professor of Chemistry and Biochemistry, Ohio State University
2015–2021	Assistant Professor of Chemistry and Biochemistry, Ohio State University
2012	Visiting Scholar at Simbios, NIH Center for Biomedical Computation, Stanford University
2011–2015	Postdoctoral Researcher in Department of Pharmacology, UCSD

SCHOLARSHIPS, HONORS, AND AWARDS

2020	Sloan Research Fellow, Alfred P. Sloan Foundation
2019	ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry
2019	Ohio State University Elizabeth L. Gross Award for Faculty Excellence
2018	National Science Foundation CAREER Award
2013	American Heart Association's Council on Basic Cardiovascular Sciences Travel Award
2013	Protein Society Finn Wold Award
2012	OpenMM Visiting Fellow Scholarship, Stanford University
2012–2014	Post-Doctoral Fellowship from American Heart Association
2012–2015	Post-Doctoral Research Fellowship from Center for Theoretical Biological Physics, UCSD
2011	PSB travel award from the National Library of Medicine
2010	Keystone Symposia Scholarship Award

SERVICE AND OUTREACH

UNIVERSITY SERVICE

Since 2021	Member, Strategic Hiring Committee, Dept. of Chemistry and Biochemistry
Since 2020	Member, Research Publicity Committee, Dept. of Chemistry and Biochemistry
Since 2019	Member, Graduate Student Recruitment Committee, Dept. of Chemistry and Biochemistry
Since 2017	Louis Stokes Alliances for Minority Participation (LSAMP) Faculty Mentor
Since 2016	Member, Allocations Committee Ohio Supercomputer Center
2015-2019	Member, Graduate Student Admissions Committee, Dept. of Chemistry and Biochemistry
Since 2015	Member, Computer Support Committee, Dept. of Chemistry and Biochemistry

Since 2015	Hosted 12 speakers for the Chemistry seminar series
2015-2019	Temporary Faculty Advisor for first year graduate students, OSU
Since 2016	First Year Graduate Student Oral Exams in Physical Chemistry (12 exams)
Since 2015	Faculty Committee Member for 2 Undergraduate Honors Thesis, 32 PhD Candidacy Exams, 37 PhD Committee Meetings, 11 PhD Defenses
2015-2017	Faculty Advisor, Physical Chemistry Student Lecture Series, OSU
2015	Review panelist for 2016 Fulbright U.S. Student Program
2009–2011	Vice President of Academic Affairs, Vanderbilt University Chemical and Physical Biology Graduate Student Association,

Research Advising:

Postdoctoral Fellows: Sumudu Leelananda, William Coldren, Sten Heinze, OSU

Graduate Students: Melanie Aprahamian, Jacob Bowman, Stephanie Kim, Justin Seffernick, Sarah Biehn, Patrick Dougherty, Austin Cool, Bargeen Turzo, Daniel Marzolf, Eric Hantz, Zach Drake, Will Higgins, Jiadi He, Paul Toth, OSU

Undergraduate Students: Cassadie Baker, Meghan Buckley, Austin Cool, Matt Belardo, OSU

PROFESSIONAL / SCIENTIFIC COMMUNITY SERVICE

2022	Organizer 52nd Midwest Theoretical Chemistry Conference. Columbus, OH
2021	Participant, NSF MCB Synthesis Planning Workshop. Virtual Format.
2020	Organizer RosettaCon 2020. Virtual Format.
2020-present	Member, Rosetta Commons Justice, Equity, Diversity, and Inclusion Committee
2019-present	Member, Rosetta Commons Executive Board
2019	Symposium Organizer "Advances in Data Collection & Analysis of Biomedical Structures" at ACS Annual Meeting 2019. Orlando, FL
2018–present	Summer REU Mentor; Kenyon College, Oberlin College, University of Michigan, Denison University, Lehigh University, College of Wooster students
2018	External Examiner at Kenyon College, OH
2018	Ad hoc Member, NIH Biophysics of Neural Systems Study Section
2017	Session Chair "Molecular Mechanics" at ACS Annual Meeting 2017. San Francisco, CA
2017	Session Chair "Molecular Dynamics II" at BPS Annual Meeting 2017. New Orleans, LA
2012	Session Chair "Molecular Mechanics" at ACS Annual Meeting 2012. San Diego, CA
2011–present	Reviewer for Chemical Reviews, Science, Nature Methods, Journal of the American Chemical Society, WIREs Computational Molecular Science, Nature Communications, Nature Protocols, Chemical Science, Journal of Medicinal Chemistry, Analytical Chemistry, Journal of Physical Chemistry Letters, Bioinformatics, Journal of Chemical Theory and Computation, PLOS Computational Biology, Journal of Molecular and Cellular Cardiology, Structure, ACS Chemical Biology, Journal of Proteome Research, Computational and Structural Biotechnology Journal, Scientific Reports, Journal of Chemical Information and Modeling, Biophysical Journal, ACS Combinatorial Science, Journal of Physical Chemistry, Chemical Biology & Drug Design, and others

COMMUNITY OUTREACH ACTIVITIES

2018	Ohio Supercomputer Center Summer Institute, Lecturer, OH High Schools, Columbus, OH
Since 2016	Breakfast of Science Champions, Laboratory host, Local Middle Schools, Columbus, OH
2012–2014	Scientific talks at middle and high schools through the San Diego Nifty Fifty Program

PROFESSIONAL AFFILIATIONS

Since 2017	Member, American Society for Mass Spectrometry
Since 2017	Faculty Mentor, Ohio State NIH Molecular Biophysics Training Program

Since 2015 Faculty Mentor, Ohio State Biochemistry Program
Since 2015 Faculty Mentor, Ohio State Biophysics Program
Since 2015 Faculty Mentor, Ohio State Chemical Physics Program
Since 2011 Member, American Heart Association
Since 2011 Member, American Chemical Society
Since 2011 Member, Protein Society
Since 2009 Member, Biophysical Society
Since 2003 Member, German Physical Society

TEACHING EXPERIENCE

Since 2015 Ohio State University, Assistant/Associate Professor

- CHEM 1210, General Chemistry 1 (undergraduate student course); Springs 2020, 2021, Autumn 2021
- CHEM 4300, Physical Chemistry 1 (undergraduate student course); Autumns 2015, 2016, 2017, 2018
- CHEM 7470, Computational Chemistry (graduate student course); Springs 2017, 2018, 2019
- OSBP 7700, Interdisciplinary Student Seminar (graduate student course); Autumn 2018
- Mentor postdocs, graduate and undergraduate students

2011–2015 University of California, San Diego, Postdoctoral Researcher

- Instructor at Simula Summer School in Computational Physiology, UCSD
- Instructor at Membrane Protein Structures by Cell-Free Synthesis, NMR Spectroscopy and Dynamics Workshop, Academia Sinica, Taipei, Taiwan
- Applied Bioinformatics (CHEM 280), Guest Lecturer, UCSD
- Instructor at National Biomedical Computational Resource Summer Institute, UCSD
- Mentored graduate and undergraduate students with Prof. Andy McCammon

2006–2011 Vanderbilt University, Graduate Researcher

- CHEM 236, Teaching Assistant for Physical Chemistry Laboratory; Fall 2007

RESEARCH SUPPORT

(PI Lindert) 01/15/2018 – 11/30/2022
NIH R01HL137015 $223,963 (direct costs to Lindert lab, Year 5)
Molecular models to characterize actions of calcium sensitizing drugs

(PI Lindert) 02/01/2018 – 01/31/2023
NSF CHE1750666 $74,270 (direct costs, Year 5)
CAREER: CDS&E: Protein structure prediction from covalent labeling MS data

(PI Lindert) 09/15/2020 - 09/14/2022
Alfred P. Sloan Foundation $75,000 (total direct costs)
Sloan Research Fellowship: Predicting protein complex structures from integrative modeling

(PI Mitton-Fry) 11/30/2019 – 11/29/2022
Falk Medical Trust $87,266 (total direct costs to Lindert Lab)

Combating antibiotic resistance with novel bacterial topoisomerase inhibitors
Role: Co-Investigator

(PI Wysocki) 07/01/2018 – 06/30/2023
NIH P41GM128577 $118,787 (direct costs to Lindert lab, Year 4)
Resource for Native Mass Spectrometry Guided Structural Biology
Role: Project-Lead

(PI Ahmer) 09/24/2018-08/31/2022
NIH R01 AI140541 $70,645 (direct costs to Lindert Lab, Year 4)
Salmonella-specific therapeutics
Role: Co-Investigator

Completed
(PI Lindert) 09/01/2017 – 05/31/2020
NIH R03AG054904 $83,072 (total direct costs to Lindert lab)
Rational drug design for chronic neuronal damage

(PI Mitton-Fry) 02/28/2018-11/27/2019
Falk Medical Trust $43,669 (total direct costs to Lindert Lab)
Novel therapies for MFSA and innovative methods for tackling bacterial resistance
Role: Co-Investigator

PRESENTATIONS

Invited Talks and Seminars

2022	Chemistry Departmental Seminar, University of New Mexico, Albuquerque, NM
2021	Institute for Drug Discovery Seminar, Leipzig University, Leipzig, Germany
2021	Chemistry Departmental Seminar, ETH Zürich, Zürich, Switzerland; virtual
2020	Laufer Center for Physical Biology Seminar, Stony Brook University, Stony Brook, NY
2019	Pharmaceutical Chemistry Departmental Seminar, Halle University, Halle, Germany
2019	Chemistry Departmental Seminar, University of Washington, Seattle, WA
2019	Chemistry Departmental Seminar, University of California, Davis, Davis, CA
2019	Chemistry Departmental Seminar, University of Florida, Gainesville, FL
2019	Physics Departmental Seminar, Georgia Institute of Technology, Atlanta, GA
2019	Pharmacology Departmental Seminar, Case Western Reserve University, Cleveland, OH
2019	Chemistry Departmental Seminar, Vanderbilt University, Nashville, TN
2019	Center for Computational Biology Seminar, University of Kansas, Lawrence, KS
2019	Biological Sciences Departmental Seminar, University of Pittsburgh, Pittsburgh, PA
2019	Chemistry Departmental Seminar, Florida A&M University, Tallahassee, FL
2018	Biochemistry Departmental Lecture Series, Leipzig University, Leipzig, Germany
2018	Chemistry Departmental Seminar, Georgia State University, Atlanta, GA
2018	Chemistry Departmental Seminar, Arizona State University, Phoenix, AZ
2018	Chemistry Departmental Seminar, Western Kentucky University, Bowling Green, KY
2018	MBTP Symposium, Ohio State University, Columbus, OH
2018	Chemistry Departmental Seminar, Duquesne University, Pittsburgh, PA
2018	Biophysics Program Seminar, Ohio State University, Columbus, OH
2017	Medicinal Chemistry & Pharmacognosy Departmental Seminar, Ohio State University, Columbus, OH
2017	MBTP/CSB Departmental Seminar, Vanderbilt University, Nashville, TN

2017 Life Sciences IGP Symposium, Ohio State University, Columbus, OH
2017 Chemistry Departmental Seminar, Hamilton College, Clinton, NY
2016 Medicinal & Biological Chemistry Departmental Seminar, University of Toledo, Toledo, OH
2016 Chemistry Departmental Seminar, Indiana University of Pennsylvania, Indiana, PA

Invited Presentations at Professional Meetings

2022 Oral Presentation at European RosettaCon, Warsaw, Poland
2022 Oral Presentation at ACS National Meeting, San Diego, CA
2021 Oral Presentation at ACS National Meeting, Atlanta, GA (virtual)
2021 Oral Presentation at Computational Tools for Native Mass Spectrometry workshop, virtual
2021 Oral Presentation at Telluride Conference on Mathematical and Computational Medicine, virtual
2019 Oral Presentation at Native Mass Spectrometry Workshop, Amherst, MA
2019 Oral Presentation at Midwest Undergraduate Computational Chemistry Consortium Conference, Columbus, OH
2019 Oral Presentation at CECAM Workshop on Multiscale Modeling, Lausanne, Switzerland
2018 Oral Presentation at ACS National Meeting, Boston, MA
2018 Oral Presentation at Bluegrass Molecular Biophysics Symposium, Lexington, KY
2017 Oral Presentation at 4th International Conference on Protein & RNA Structure Prediction, Montego Bay, Jamaica
2017 Oral Presentation at ACS National Meeting, Washington, DC

Contributed Presentations at Professional Meetings

2022 Poster Presentation at Biophysical Society Annual Meeting, San Francisco, CA
2021 Oral Presentation at Tandem Mass Spectrometry Workshop, Lake Louise, Alberta, Canada
2019 Oral Presentation at Tandem Mass Spectrometry Workshop, Lake Louise, Alberta, Canada
2019 Poster Presentation at Basic Cardiovascular Sciences Scientific Sessions, Boston, MA
2019 Oral Presentation at Advancing Mass Spectrometry conference, Amherst, MA
2019 Poster Presentation at Advancing Mass Spectrometry conference, Amherst, MA
2019 Oral Presentation at ACS National Meeting, Orlando, FL
2019 Poster Presentation at ACS National Meeting, Orlando, FL
2019 Poster Presentation at Biophysical Society Annual Meeting, Baltimore, MD
2018 Oral Presentation at ASMS National Meeting, San Diego, CA
2018 Oral Presentation at ISHR Annual Meeting, Halifax, NS
2018 Poster Presentation at ISHR Annual Meeting, Halifax, NS
2018 Oral Presentation at Myofilament Meeting, Madison, WI
2018 Poster Presentation at Myofilament Meeting, Madison, WI
2018 Poster Presentation at Biophysical Society Annual Meeting, San Francisco, CA
2018 Oral Presentation at ASMS Sanibel Conference, St. Petersburg, FL
2018 Poster Presentation at ASMS Sanibel Conference, St. Petersburg, FL
2017 Poster Presentation at Advancing Mass Spectrometry conference, Ann Arbor, MI
2017 Poster Presentation at ASMS National Meeting, Indianapolis, IN
2017 Oral Presentation at ACS National Meeting, San Francisco, CA
2017 Oral Presentation at Biophysical Society Annual Meeting, New Orleans, LA
2016 Oral Presentation at Symposium on Biomolecular Structure, Dynamics and Function, Providence, RI
2016 Oral Presentation at ACS National Meeting, San Diego, CA
2016 Oral Presentation at Biophysical Society Annual Meeting, Los Angeles, CA

PATENTS

1. Wei Zhu, **Steffen Lindert**, Yonghui Zhang, William Sinko, Kai Li, James Andrew McCammon, Eric Oldfield; "Antibacterial compounds targeting isoprenoid biosynthesis" US patent #US9,951,097B2, Issued 04/24/2018

PEER-REVIEWED PUBLICATIONS

Independent career

73. Khaje, N.A.; Eletsky, A.; Biehn, S.E.; Mobley, C.K.; Rogals, M.J.; Kim, Y.; Mishra, S.K.; Doerksen, R.J.; **Lindert, S.**; Prestegard, J.H.; Sharp, J.S. (2022), Validated determination of NRG1 Ig-like domain structure by mass spectrometry coupled with computational modeling. Commun Biol 5 (1), 452.
72. Biehn, S.E.; Picarello, D.M., Pan, X.; Vachet, R.W.; **Lindert, S.** (2022), Accounting for Neighboring Residue Hydrophobicity in Diethylpyrocarbonate Labeling Mass Spectrometry Improves Rosetta Protein Structure Prediction. J Am Soc Mass Spectrom 33 (3), 584-591.
71. Nguyen, T.T.; Marzolf, D.R.; Seffernick, J.T.; Heinze, S.; **Lindert, S.** (2022), Protein structure prediction using residue-resolved protection factors from hydrogen-deuterium exchange NMR. Structure 30 (2), 313-320.
70. Biehn, S.E.; **Lindert, S.** (2022), Protein Structure Prediction with Mass Spectrometry Data. Annu Rev Phys Chem. 73, 1-19.
69. Lu, Y.; Vibhute, S.; Li, L.; Okumu, A.; Ratigan, S.C.; Nolan, S.; Papa, J.L.; Mann, C.A.; English, A.; Chen, A.; Seffernick, J.T.; Koci, B.; Duncan, L.R.; Roth, B.; Cummings, J.E.; Slayden, R.A.; **Lindert, S.**; McElroy, C.A.; Wozniak, D.J.; Yalowich, J.; Mitton-Fry, M.J. (2021), Optimization of TopoIV Potency, ADMET Properties, and hERG Inhibition of 5-Amino-1,3-dioxane-Linked Novel Bacterial Topoisomerase Inhibitors: Identification of a Lead with In Vivo Efficacy against MRSA. J Med Chem 64 (20), 15214-15249.
68. Cool, A.M.; **Lindert, S.** (2021), Computational Methods Elucidate Consequences of Mutations and Post-translational Modifications on Troponin I Effective Concentration to Troponin C. J Phys Chem B 125 (27), 7388-7396.
67. Hantz, E.R.; **Lindert, S.** (2021), Adaptive Steered Molecular Dynamics Study of Mutagenesis Effects on Calcium Affinity in the Regulatory Domain of Cardiac Troponin C. J Chem Inf Model 61 (6), 3052-3057.
66. Biehn, S.E.; Limpikirati, P.; Vachet, R.W.; **Lindert, S.** (2021), Utilization of Hydrophobic Microenvironment Sensitivity in Diethylpyrocarbonate Labeling for Protein Structure Prediction. Anal Chem 93 (23), 8188-8195.
65. Seffernick, J.T.; Canfield, S.M.; Harvey, S.R.; Wysocki, V.H.; **Lindert, S.** (2021), Prediction of Protein Complex Structure Using Surface-Induced Dissociation and Cryo-Electron Microscopy. Anal Chem 93 (21), 7596–7605.
64. Marzolf, D.R.; Seffernick, J.T.; **Lindert, S.** (2021), Protein Structure Prediction from NMR Hydrogen-Deuterium Exchange Data. J Chem Theory Comput 17 (4), 2619-2629.
63. Rayani, K.; Seffernick, J.T.; Li, A.Y.; Davis, J.P.; Spuches, A.M.; Van Petegem, F.; Solaro, R.J.; **Lindert, S.**; Tibbits, G.F. (2021), Binding of calcium and magnesium to human cardiac Troponin C. J Biol Chem 296, 100350.
62. Biehn, S.E.; **Lindert, S.** (2021), Accurate Protein Structure Prediction with Hydroxyl Radical Protein Footprinting Data. Nat Commun 12, 341.
61. Kim, S.S.; Alves, M.J.; Gygli, P.; Otero, J.; **Lindert, S.** (2021), Identification of novel cyclin A2 binding site and nanomolar inhibitors of cyclin A2-CDK2 complex. Curr Comput Aided Drug Des 17 (1), 57-68.
60. Seffernick, J.T.; **Lindert, S.** (2020), Hybrid methods for combined experimental and computational determination of protein structure. J Chem Phys 153 (24), 240901.

59. Lu, Y.; Papa, J.L.; Nolan, S.; English, A.; Seffernick, J.T.; Shkolnikov, N.; Powell, J.; **Lindert, S.**; Wozniak, D.J.; Yalowich, J.; Mitton-Fry, M.J. (2020), Dioxane-Linked Amide Derivatives as Novel Bacterial Topoisomerase Inhibitors against Gram-Positive Staphylococcus aureus. ACS Med Chem Lett 11 (12), 2446-2454.
58. Coldren, W.H.; Tikunova, S.B.; Davis, J.P.; **Lindert, S.** (2020), Discovery of Novel Small-Molecule Calcium Sensitizers for Cardiac Troponin C: A Combined Virtual and Experimental Screening Approach. J Chem Inf Model 60 (7), 3648-3661.
57. Leman, J.K.; Weitzner, B.D.; Lewis, S.M.; Adolf-Bryfogle, J.; Alam, N.; Alford, R.F.; Aprahamian, M.; Baker, D.; Barlow, K.A.; Barth, P.; Basanta, B.; Bender, B.J.; Blacklock, K.; Bonet, J.; Boyken, S.E.; Bradley, P.; Bystroff, C.; Conway, P.; Cooper, S.; Correia, B.E.; Coventry, B.; Das, R.; De Jong, R.M.; DiMaio, F.; Dsilva, L.; Dunbrack, R.; Ford, A.S.; Frenz, B.; Fu, D.Y.; Geniesse, C.; Goldschmidt, L.; Gowthaman, R.; Gray, J.J.; Gront, D.; Guffy, S.; Horowitz, S.; Huang, P.S.; Huber, T.; Jacobs, T.M.; Jeliazkov, J.R.; Johnson, D.K.; Kappel, K.; Karanicolas, J.; Khakzad, H.; Khar, K.R.; Khare, S.D.; Khatib, F.; Khramushin, A.; King, I.C.; Kleffner, R.; Koepnick, B.; Kortemme, T.; Kuenze, G.; Kuhlman, B.; Kuroda, D.; Labonte, J.W.; Lai, J.K.; Lapidoth, G.; Leaver-Fay, A.; **Lindert, S.**; Linsky, T.; London, N.; Lubin, J.H.; Lyskov, S.; Maguire, J.; Malmström, L.; Marcos, E.; Marcu, O.; Marze, N.A.; Meiler, J.; Moretti, R.; Mulligan, V.K.; Nerli, S.; Norn, C.; Ó'Conchúir, S.; Ollikainen, N.; Ovchinnikov, S.; Pacella, M.S.; Pan, X.; Park, H.; Pavlovicz, R.E.; Pethe, M.; Pierce, B.G.; Pilla, K.B.; Raveh, B.; Renfrew, P.D.; Burman, S.S.R.; Rubenstein, A.; Sauer, M.F.; Scheck, A.; Schief, W.; Schueler-Furman, O.; Sedan, Y.; Sevy, A.M.; Sgourakis, N.G.; Shi, L.; Siegel, J.B.; Silva, D.A.; Smith, S.; Song, Y.; Stein, A.; Szegedy, M.; Teets, F.D.; Thyme, S.B.; Wang, R.Y.; Watkins, A.; Zimmerman, L.; Bonneau, R. (2020), Macromolecular Modeling and Design in Rosetta: Recent Methods and Frameworks. Nat Methods 17 (7), 665-680.
56. Leelananda, S.P.; **Lindert, S.** (2020), Using NMR Chemical Shifts and Cryo-EM Density Restraints in Iterative Rosetta-MD Protein Structure Refinement. J Chem Inf Model 60 (5), 2522-2532.
55. Sengupta, A.; Wu, J.; Seffernick, J.T.; Sabag-Daigle, A.; Thomsen, N.; Chen, T.H.; Di Capua, A.; Bell, C.E.; Ahmer, B.M.M.; **Lindert, S.**; Wysocki, V.H.; Gopalan, V. (2019), Integrated use of biochemical, native mass spectrometry, computational and genome-editing methods to elucidate the mechanism of a Salmonella deglycase. J Mol Biol 431 (22), 4497-4513.
54. Bowman, J.D.; **Lindert, S.** (2019), Computational Studies of Cardiac and Skeletal Troponin. Front Mol Biosci. Front Mol Biosci 6:68.
53. Seffernick, J.T.; Ren, H.; Kim, S.S.; **Lindert, S.** (2019), Measuring Intrinsic Disorder and Tracking Conformational Transitions Using Rosetta ResidueDisorder. J Phys Chem B 123 (33), 7103-7112.
52. Seffernick, J.T.; Harvey, S.R.; Wysocki, V.H.; **Lindert, S.** (2019), Predicting Protein Complex Structure from Surface-Induced Dissociation Mass Spectrometry Data. ACS Cent Sci 5 (8), 1330-1341.
51. Bowman, J.D.; Coldren, W.H.; **Lindert, S.** (2019), Mechanism of Cardiac Troponin C Calcium Sensitivity Modulation by Small Molecules Illuminated by Umbrella Sampling Simulations. J Chem Inf Model 59 (6), 2964-2972.
50. Li, L.; Okumu, A.A.; Nolan, S.; English, A.; Vibhute, S.; Lu, Y.; Hervert-Thomas, K.; Seffernick, J.T.; Azap, L.; Cole, S.L.; Shinabarger, D.; Koeth, L.; **Lindert, S.**; Yalowich, J.; Wozniak, D.J.; Mitton-Fry, M.J. (2019), 1,3-Dioxane-linked Bacterial Topoisomerase Inhibitors with Enhanced Antibacterial Activity and Reduced hERG Inhibition. ACS Infect Dis 5 (7), 1115-1128.
49. Aprahamian, M.L.; **Lindert, S.** (2019), Utility of Covalent Labeling Mass Spectrometry Data in Protein Structure Prediction with Rosetta. J Chem Theory Comput 15 (5), 3410-3424.
48. Harvey, S.R.; Seffernick, J.T.; Quintyn, R.S.; Song, Y.; Ju, Y.; Yan, J.; Sahasrabuddhe, A.N.; Norris, A.; Zhou, M.; Behrman, E.J.; **Lindert, S.**; Wysocki, V.H. (2019), Relative interfacial

cleavage energetics of protein complexes revealed by surface collisions. Proc Natl Acad Sci U S A 116 (17), 8143-8148.

47. Kim, S.S.; Aprahamian, M.L.; **Lindert, S.** (2019), Improving inverse docking target identification with Z-score selection. Chem Biol Drug Des 93 (6), 1105-1116.
46. Rhodes, C.A.; Dougherty, P.G.; Cooper, J.K.; Qian, Z.; **Lindert, S.**; Wang, Q.E.; Pei, D. (2018), Cell-Permeable Bicyclic Peptidyl Inhibitors against NEMO-IκB kinase Interaction Directly from a Combinatorial Library. J Am Chem Soc 140 (38), 12102–12110.
45. Bowman, J.D.; **Lindert, S.** (2018), Molecular Dynamics and Umbrella Sampling Simulations Elucidate Differences in Troponin C Isoform and Mutant Hydrophobic Patch Exposure. J Phys Chem B 122 (32), 7874–7883.
44. Aprahamian, M.L.; Chea, E.E.; Jones, L.M.; **Lindert, S.** (2018), Rosetta Protein Structure Prediction from Hydroxyl Radical Protein Footprinting Mass Spectrometry Data. Anal Chem 90 (12), 7721–7729.
43. Kim, S.S.; Seffernick, J.T.; **Lindert, S.** (2018), Accurately Predicting Disordered Regions of Proteins Using Rosetta ResidueDisorder Application. J Phys Chem B 122 (14), 3920-30.
42. Aprahamian, M.L.; Tikunova, S.B.; Price, M.V.; Cuesta, A.F.; Davis, J.P.; **Lindert, S.** (2017), Successful Identification of Cardiac Troponin Calcium Sensitizers Using a Combination of Virtual Screening and ROC Analysis of Known Troponin C Binders. J Chem Inf Model 57 (12), 3056-3069.
41. Leelananda, S.P.; **Lindert, S.** (2017), Iterative Molecular Dynamics-Rosetta Membrane Protein Structure Refinement Guided by Cryo-EM Densities. J Chem Theory Comput 13 (10), 5131-5145.
40. Schwebach, C.L.; Agrawal, R.; **Lindert, S.**; Kudryashova, E.; Kudryashov, D.S. (2017), The Roles of Actin-Binding Domains 1 and 2 in the Calcium-Dependent Regulation of Actin Filament Bundling by Human Plastins. J Mol Biol 429 (16), 2490-508.
39. Leelananda, S.P.; **Lindert, S.** (2016), Computational methods in drug discovery. Beilstein J Org Chem 12, 2694–2718.
38. Cai, F.; Li, M.X.; Pineda-Sanabria, S.E.; Gelozia, S.; **Lindert, S.**; West, F., et al. (2016) Structures reveal details of small molecule binding to cardiac troponin. J Mol Cell Cardiol 101, 134-44.
37. Cheng, Y.; **Lindert, S.**; Oxenford, L.; Tu, A.Y.; McCulloch, A.D.; Regnier, M. (2016) Effects of Cardiac Troponin I Mutation P83S on Contractile Properties and the Modulation by PKA-Mediated Phosphorylation. J Phys Chem B 120 (33), 8238-53.
36. Dewan, S.; McCabe, K.J.; Regnier, M.; McCulloch, A.D.; **Lindert, S.** (2016), Molecular Effects of cTnC DCM Mutations on Calcium Sensitivity and Myofilament Activation-An Integrated Multiscale Modeling Study. J Phys Chem B 120 (33), 8264-75.
35. Feng, X.; Zhu, W.; Schurig-Briccio, L.A.; **Lindert, S.**; Shoen, C.; Hitchings, R.; Li, J.; Wang, Y.; Baig, N.; Zhou, T.; Kim, B.K.; Crick, D.C.; Cynamon , M.; McCammon, J. A.; Gennis , R.B.; Oldfield, E. (2015), Antiinfectives targeting enzymes and the proton motive force. Proc Natl Acad Sci U S A 112 (51), E7073-E7082.

<u>Prior to OSU</u>

34. Cheng, Y.; Rao, V. S.; Tu, A.Y.; **Lindert, S.**; Wang, D.; Oxenford, L.; McCulloch, A. D.; McCammon, J. A.; Regnier, M. (2015), Troponin I Mutations R146G and R21C Alter Cardiac Troponin Function, Contractile Properties, and Modulation by Protein Kinase A (PKA)-mediated Phosphorylation. J Biol Chem 290 (46), 27749-27766.
33. **Lindert, S.**; McCammon, J. A. (2015), Improved cryoEM-Guided Iterative Molecular Dynamics-Rosetta Protein Structure Refinement Protocol for High Precision Protein Structure Prediction. J Chem Theory Comput 11 (3), 1337-1346.
32. Kim, M. O.; Feng, X.; Feixas, F.; Zhu, W.; **Lindert, S.**; Bogue, S.; Sinko, W.; de Oliveira, C.; Rao, G.; Oldfield, E.; McCammon, J. A. (2015), A Molecular Dynamics Investigation of

Mycobacterium tuberculosis Prenyl Synthases: Conformational Flexibility and Implications for Computer-aided Drug Discovery. Chem Biol Drug Des 85 (6), 756-69.
31. **Lindert, S.**; Cheng, Y.; Kekenes-Huskey, P. M.; Regnier, M.; McCammon, J. A. (2015), Effects of HCM cTnI Mutation R145G on Troponin Structure and Modulation by PKA Phosphorylation elucidated by Molecular Dynamics Simulations. Biophys J 108 (2), 395–407.
30. **Lindert, S.***; Tallorin, L. C.*; Nguyen, Q. G.; Burkart, M.D.; McCammon, J. A. (2015), In silico Screening for Plasmodium falciparum Enoyl-ACP Reductase inhibitors. J Comput Aided Mol Des 29 (1), 79-87.
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