

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

- 2024 OSU College of Arts and Sciences Mid-Career Faculty Excellence Award
2023 Ohio State University Scarlet and Gray Associate Professor Award
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

- 2023-2024 Member, Search Committee, Physical Chemistry Faculty Position
Since 2023 Member, Curriculum Committee, OSBP graduate program
2021-2022 Member, Strategic Hiring Committee, Dept. of Chemistry and Biochemistry
2020-2022 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 15 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 (17 exams)
 Since 2015 Faculty Committee Member for 3 Undergraduate Honors Thesis, 49 PhD Candidacy Exams, 71 PhD Committee Meetings, 27 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, Elijah Day, Bryan Perez Soto, Akshaya Narayanasamy, Mac Bolz, Insha Malayil, Viraj Rana, OSU
 Undergraduate Students: Cassadie Baker, Meghan Buckley, Austin Cool, Matt Belardo, OSU

PROFESSIONAL / SCIENTIFIC COMMUNITY SERVICE

2024 Member, Admissions Committee, Rosetta Post-Baccalaureate Training Program
 2024 Ad hoc Reviewer, NSF Molecular Biophysics (BIO/MCB)
 Since 2023 Treasurer, Rosetta Commons Executive Board
 2023 Direct Submission Editor for PNAS
 2023 Session Chair “Advances in MS” at ACS Annual Meeting 2023. Indianapolis, IN
 2022 Organizer 52nd Midwest Theoretical Chemistry Conference. Columbus, OH
 2022 Participant, NSF MCB Synthesis Planning Workshop. Virtual Format.
 2020 Organizer RosettaCon 2020. Virtual Format.
 2020-2022 Member, Rosetta Commons Justice, Equity, Diversity, and Inclusion Committee
 2019-2021 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, University of Notre Dame, Towson University, Maryville College 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, ACS Central Science, Journal of the American Chemical Society, WIREs Computational Molecular Science, Nature Communications, Nature Protocols, PNAS, Cell Systems, 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, ACS Medicinal

Chemistry Letters, 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, Autumns 2021, 2022
- CHEM 4300, Physical Chemistry 1 (undergraduate student course); Autumns 2015, 2016, 2017, 2018, 2023, Spring 2024
- CHEM 6520, Thermodynamics (graduate student course); Autumn 2023
- 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) 05/15/2023 – 07/31/2026
NSF CHE2247002 \$82,803 (direct costs, Year 1)

Computational Studies to Improve Understanding and Outcomes of Covalent Labeling Mass Spectrometry Measurements

(PI Lindert) 01/15/2018 – 11/30/2024
NIH R01HL137015 \$223,963 (direct costs to Lindert lab, Year 5)
Molecular models to characterize actions of calcium sensitizing drugs

(PI Lindert) 09/15/2020 – 09/14/2025
Alfred P. Sloan Foundation \$75,000 (total direct costs)
Sloan Research Fellowship: Predicting protein complex structures from integrative modeling

(PI Mitton-Fry) 12/05/2022 – 11/30/2027
NIH R01 AI173072 \$35,309 (direct costs to Lindert Lab, Year 1)
Overcoming Resistance to Novel Bacterial Topoisomerase Inhibitors
Role: Co-Investigator

(PI Gray) 08/01/2022 – 07/31/2026
NSF MCB 2216011 \$131,813 (direct costs to Lindert Lab, Year 3+4)
RaMP: Post-Baccalaureate Training Program in Biomolecular Structure Prediction and Design
Role: Mentor

(PI Wysocki) 07/01/2023 – 06/30/2028
NIH RM1GM149374 \$126,516 (direct costs to Lindert lab, Year 1)
Native Mass Spectrometry Guided Structural Biology Center
Role: Co-Investigator

(PI Sharp) 09/01/2023 – 08/31/2027
NIH R01 GM127267 \$77,276 (direct costs to Lindert Lab, Year 1)
Molecular Structure Determination by Mass Spectrometry and Computational Modeling
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

(PI Mitton-Fry) 11/30/2019 – 11/29/2022
Falk Medical Trust \$100,469 (total direct costs to Lindert Lab)
Combating antibiotic resistance with novel bacterial topoisomerase inhibitors
Role: Co-Investigator

(PI Ahmer) 08/15/2018 – 07/31/2023
NIH R01 AI140541 \$70,645 (direct costs to Lindert Lab, Year 4)
Salmonella-specific therapeutics
Role: Co-Investigator

(PI Wysocki) 07/01/2018 – 06/30/2023
NIH P41GM128577 \$118,787 (direct costs to Lindert lab, Year 5)
Resource for Native Mass Spectrometry Guided Structural Biology
Role: Project-Lead

(PI Lindert) 02/01/2018 – 01/31/2024
NSF CHE1750666 \$74,270 (direct costs, Year 5)
CAREER: CDS&E: Protein structure prediction from covalent labeling MS data

PRESENTATIONS

Invited Talks and Seminars

2023 Center for Structural Mass Spectrometry Seminar, Halle University, Halle, Germany
2023 Chemistry Departmental Seminar, University of Girona, Girona, Spain
2023 In Silico Discovery Departmental Seminar, Janssen Pharmaceuticals; virtual
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

2023 Oral Presentation at Advancing Mass Spectrometry Conference, Austin, TX
2023 Oral Presentation at CADD Gordon Research Conference, West Dover, VT
2023 Oral Workshop Presentation at ASMS National Meeting, Houston, TX

2022 Oral Presentation at WATOC 2022, Vancouver, British Columbia, Canada
2022 Oral Presentation at Telluride Conference on Mathematical and Computational Medicine, Telluride, CO
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

2023 Oral Presentation at Tandem Mass Spectrometry Workshop, Lake Louise, Alberta, Canada
2023 Poster Presentation at European Biophysics Meeting, Stockholm, Sweden
2023 Oral Presentation at ACS MedChem Frontiers Symposium, Boston, MA
2023 Poster Presentation at ASMS National Meeting, Houston, TX
2023 Oral Presentation at Chemical Biophysics Symposium, Toronto, Ontario, Canada
2023 Oral Presentation at ACS National Meeting, Indianapolis, IN
2022 Oral Presentation at ASMS National Meeting, Minneapolis, MN
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

88. Higgins, W.T.; Vibhute, S.; Bennett, C.; **Lindert, S.** (2024), Discovery of Nanomolar Inhibitors for Human Dihydroorotate Dehydrogenase Using Structure-Based Drug Discovery Methods. *J Chem Inf Model* 64 (2), 435-448.
87. Turzo, S.B.A.; Seffernick, J.T.; Lyskov, S.; **Lindert, S.** (2023), Predicting ion mobility collision cross sections using projection approximation with ROSIE-PARCS webserver. *Brief Bioinform* 24 (5), bbad308.
86. Kovvali, S.; Gao, Y.; Cool, A.M.; **Lindert, S.**; Wysocki, V.H.; Bell, C.E.; Gopalan, V. (2023), Insights Into The Catalytic Mechanism of A Bacterial Deglycase Essential For Utilization of Fructose-Lysine. *Protein Sci* 32 (7), e4695.
85. Cool, A.M.; **Lindert, S.** (2023), Umbrella Sampling Simulations of Cardiac Thin Filament Reveal Thermodynamic Consequences of Troponin I Inhibitory Peptide Mutations. *J Chem Inf Model* 63 (11), 3534-3543.
84. Hantz, E.R.; Tikunova, S.B.; Belevych, N.; Davis, J.P.; Reiser, P. J.; **Lindert, S.** (2023), Targeting Troponin C with Small Molecules Containing Diphenyl Moieties: Calcium Sensitivity Effects on Striated Muscles and Structure-Activity Relationship. *J Chem Inf Model* 63 (11), 3462-3473.
83. Drake, Z.C.; Seffernick, J.T.; **Lindert, S.** (2022), Protein complex prediction using Rosetta, AlphaFold, and mass spectrometry covalent labeling. *Nat Commun* 13 (1), 7846.
82. Hantz, E.R.; **Lindert, S.** (2022), Computational Exploration and Characterization of Potential Calcium Sensitizing Mutations in Cardiac Troponin C. *J Chem Inf Model* 62 (23), 6201-6208.
81. Hantz, E.R.; **Lindert, S.** (2022), Actives-Based Receptor Selection Strongly Increases the Success Rate in Structure-Based Drug Design and Leads to Identification of 22 Potent Cancer Inhibitors. *J Chem Inf Model* 62 (22), 5675-5687.
80. Turzo, S.B.A.; Hantz, E.R.; **Lindert, S.** (2022), Applications of machine learning in computer-aided drug discovery. *QRB Discov* 3, e14.
79. Thirugnanasambantham, P.; Kovvali, S.; Cool, A.M.; Gao, Y.; Sabag-Daigle, A.; Boulanger, E.F.; Mitton-Fry, M.J.; Capua, A.D.; Behrman, E.J.; Wysocki, V.H.; **Lindert, S.**; Ahmer, B.M.M.; Gopalan, V. (2022), Serendipitous Discovery of a Competitive Inhibitor of FraB, a Salmonella Deglycase and Drug Target. *Pathogens* 11 (10), 1102.
78. Cool, A.M.; **Lindert, S.** (2022), Umbrella Sampling Simulations Measure Switch Peptide Binding and Hydrophobic Patch Opening Free Energies in Cardiac Troponin. *J Chem Inf Model* 62 (22), 5666-5674.
77. He, J.; Turzo, S.B.A.; Seffernick, J.T.; Kim, S.S.; **Lindert, S.** (2022), Prediction of Intrinsic Disorder Using Rosetta ResidueDisorder and AlphaFold2. *J Phys Chem B* 126 (42), 8439-8446.
76. Turzo, S.B.A.; Seffernick, J.T.; Rolland, A.D.; Donor, M.T.; Heinze, S.; Prell, J.S.; Wysocki, V.H.; **Lindert, S.** (2022), Protein shape sampled by ion mobility mass spectrometry consistently improves protein structure prediction. *Nat Commun* 13 (1), 4377.
75. Rayani, K.; Hantz, E.R.; Haji-Ghassemi, O.; Li, A.Y.; Spuches, A.M.; Van Petegem, F.; Solaro, R.J.; **Lindert, S.**; Tibbits, G.F. (2022), The effect of Mg²⁺ on Ca²⁺ binding to cardiac troponin C in hypertrophic cardiomyopathy associated TNNC1 variants. *FEBS J* 289 (23), 7446-7465.

74. Seffernick, J.T.; Turzo, S.B.A.; Harvey, S.R.; Kim, Y.; Somogyi, Á.; Marciano, S.; Wysocki, V.H.; **Lindert, S.** (2022), Simulation of Energy-Resolved Mass Spectrometry Distributions from Surface-Induced Dissociation. *Anal Chem* 94 (29), 10506-10514.
73. Khaje, N.A.; Eletsy, 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.; Jeliaskov, 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.
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* signifies equal contribution