Steffen Lindert

ADDRESS:

Office
Ohio State University
100 W. 18th. Ave.
2114 Newman & Wolfrom Laboratory
Columbus, OH 43210
Phone: (614) xxx-xxxx
Fax: (614) xxx-xxxx
Email: lindert.1@osu.edu
Website: http://users.mccammon.ucsd.edu/~slindert/

Home
283 E 1st Ave, Suite 215
Columbus, OH 43215
Phone: (615) 438-3523
Email: steffen.lindert@gmail.com

EDUCATION:

2006-2010 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, WORK EXPERIENCE:

2015–present 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
2006–2010 Graduate Student in Chemical and Physical Biology, Vanderbilt University School of Medicine
2005–2006 Master thesis research in Biophysics, University of Leipzig, Germany
2005 Student worker at Siemens Corporate Technologies, Munich, Germany (Simulation of Piezoelectric Injection Pumps)
2003–2004 Student worker at University of Leipzig, Germany (translation of lab manuals into English)
2002–2003 Undergraduate research assistant in semiconductor physics, University of Edinburgh

SCHOLARSHIPS, HONORS, AND AWARDS:

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 (Percentile Rank: 2.46; Score: 1.34, with 1.0-1.4 being considered 'excellent')

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
2008 Best poster Frontiers in Macromolecular Simulations Symposium, Birmingham, AL

INVITED LECTURES:

2014 Finding novel anticancer and antibacterial drug leads using CADD - FPPS and UPPS inhibitors from *in silico* screening. Telluride Science Research Center Meeting on Molecular Recognition. Telluride, CO
2014 Computational Methods for Protein Structure Prediction, Protein Dynamics and Drug Discovery. Invited Seminar. University of Wisconsin. Milwaukee, WI
2014 Computational Methods for Protein Structure Prediction, Protein Dynamics and Drug Discovery. Invited Seminar. Colorado State University. Fort Collins, CO
2014 Computational Methods for Protein Structure Prediction, Protein Dynamics and Drug Discovery. Invited Seminar. Virginia Tech. Blacksburg, VA
2013 Computational Methods for Protein Structure Prediction, Protein Dynamics and Drug Discovery. Invited Seminar. Baylor College of Medicine. Houston, TX
2013 Iterative Molecular Dynamics – Rosetta protein structure refinement protocol. RosettaCon 2013. Leavenworth, WA
2013 Calcium binding to Troponin C is crucial to Muscle Contraction – A Computational Perspective. Invited Seminar. University of Utah. Salt Lake City, UT
2012 Dynamics and Calcium Association to the N-Terminal Regulatory Domain of Human Cardiac Troponin C: A Multiscale Computational Study. Symposium of Biomolecular Structure, Dynamics and Function. Memphis, TN
2012 Molecular Dynamics and Calcium Binding Studies on Troponin C. ACS Annual Meeting 2012. San Diego, CA
2012 Molecular Dynamics and Calcium Binding Studies on Troponin C. Biophysical Society Annual Meeting 2012. San Diego, CA
2011 Building ab-initio models with EM-Fold. Pacific Symposium on Biocomputing 2011. Big Island, HI
2010 Rosetta refinement in medium resolution density maps reaches atomic resolution for proteins of up to 350 residues. RosettaCon 2010. Leavenworth, WA
2010 BCL::EM-Fold: Protein Folding Tool for Medium Resolution Density Maps. Keystone Symposium Structural Biology. Breckenridge, CO
2009 Folding Proteins into Medium Resolution CryoEM Density Maps. Frontiers in Macromolecular Simulations Symposium. Atlanta, GA

PEER-REVIEWED PUBLICATIONS:

1. **Lindert, S.**, Stewart, P.L., and Meiler, J. (2009). Hybrid approaches: applying computational methods in cryo-electron microscopy. Curr Opin Struct Biol *19*, 218-225.

2. **Lindert, S.**, Staritzbichler, R., Wotzel, N., Karakas, M., Stewart, P.L., and Meiler, J. (2009). EM-Fold: De novo folding of alpha-helical proteins guided by intermediate-resolution electron microscopy density maps. Structure *17*, 990-1003.

3. **Lindert, S.**, Silvestry, M., Mullen, T.M., Nemerow, G.R., and Stewart, P.L. (2009). Cryo-electron microscopy structure of an adenovirus-integrin complex indicates conformational changes in both penton base and integrin. J Virol *83*, 11491-11501.

4. Silvestry, M., **Lindert, S.**, Smith, J.G., Maier, O., Wiethoff, C.M., Nemerow, G.R., and Stewart, P.L. (2009). Cryo-electron microscopy structure of adenovirus type 2 temperature-sensitive mutant 1 reveals insight into the cell entry defect. J Virol *83*, 7375-7383.

5. Smith, J. G.; Silvestry, M.; **Lindert, S.**; Lu, W.; Nemerow, G. R.; Stewart, P. L. (2010), Insight into the mechanisms of adenovirus capsid disassembly from studies of defensin neutralization. PLoS Pathog 2010, 6 (6), e1000959

6. Woetzel, N., **Lindert, S.**, Stewart, P.L., and Meiler, J. (2011). BCL::EM-Fit: rigid body fitting of atomic structures into density maps using geometric hashing and real space refinement. Journal of Structural Biology *175*, 264-276.

7. **Lindert, S.**, Alexander, N., Wotzel, N., Karakas, M., Stewart, P.L., and Meiler, J. (2012). EM-Fold: De Novo Atomic-Detail Protein Structure Determination from Medium-Resolution Density Maps. Structure *20*, 464-478.
   Article featured in PSI Nature Structural Biology KB: http://kb.psi-structuralgenomics.org/update/2012/05/full/sbkb.2011.79.html

8. **Lindert, S.**, Hofmann, T., Wotzel, N., Karakas, M., Stewart, P.L., and Meiler, J. (2012). Ab initio protein modeling into CryoEM density maps using EM-Fold. Biopolymers 97, 669-677.

9. **Lindert, S.***, Durrant, J.*, McCammon, JA. (2012). LigMerge: A Fast Algorithm to Generate Models of Novel Potential Ligands from Sets of Known Binders. Chem Biol Drug Des 80, 358-365.

10. **Lindert, S.**, Kekenes-Huskey, P.M., Huber, G., Pierce, L., and McCammon, J.A. (2012). Dynamics and calcium association to the N-terminal regulatory domain of human cardiac troponin C: a multiscale computational study. J Phys Chem B 116, 8449-8459.

11. **Lindert, S.** and McCammon, J.A. (2012). Dynamics of Plasmodium falciparum enoyl-ACP reductase and implications on drug discovery. Protein Sci 21(11): 1734-1745.

12. **Lindert, S.**; Kekenes-Huskey, P. M.; McCammon, J. A. (2012). Long-timescale molecular dynamics simulations elucidate the dynamics and kinetics of exposure of the hydrophobic patch in troponin C. Biophys J 103 (8), 1784-1789.

13. Kekenes-Huskey, P. M., **Lindert, S.** and McCammon, J.A. (2012). Molecular basis of calcium-sensitizing and desensitizing mutations of the human cardiac troponin C regulatory domain: a multi-scale simulation study. PLoS Comput Biol 8 (11), e1002777.

14. **Lindert, S.**; Stewart, P. L.; Meiler, J. (2013), Computational determination of the orientation of a heat repeat-like domain of DNA-PKcs. Comput Biol Chem 42, 1-4.

15. Sinko, W.; **Lindert, S.**; McCammon, J. A. (2013), Accounting for Receptor Flexibility and Enhanced Sampling Methods in Computer-Aided Drug Design. Chem Biol Drug Des 81 (1), 41-49.

16. Zhu, W.; Zhang, Y.; Sinko, W.; Hensler, M. E.; Olson, J.; Molohon, K. J.; **Lindert, S.**; Cao, R.; Li, K.; Wang, K.; Wang, Y.; Liu, Y. L.; Sankovsky, A.; de Oliveira, C. A.; Mitchell, D. A.; Nizet,

V.; McCammon, J. A.; Oldfield, E. (2013), Antibacterial drug leads targeting isoprenoid biosynthesis. Proc Natl Acad Sci U S A 110 (1), 123-128.

17. **Lindert, S.**; Zhu, W.; Liu, Y. L.; Pang, R.; Oldfield, E.; McCammon, J.A. (2013), Farnesyl diphosphate synthase inhibitors from in silico screening. Chem Biol Drug Des 81 (6), 742-8.

18. Timson, D.; **Lindert, S.** (2013), Comparison of Dynamics of Wildtype and V94M Human UDP-Galactose 4-Epimerase - A computational perspective on severe Epimerase-deficiency Galactosemia. Gene 526 (2), 318-24.

19. Durrant, J. D.; **Lindert, S.**; McCammon, J. A. (2013), AutoGrow 3.0: An improved algorithm for chemically tractable, semi-automated protein inhibitor design. J Mol Graph Model 44C, 104-112.

20. **Lindert, S.**; Meiler, J.; McCammon, J. A. (2013), Iterative Molecular Dynamics – Rosetta protein structure refinement protocol to improve model quality. J Chem Theory Comput 9(8), 3843-7.

21. **Lindert, S.**; Bucher, D.; Eastman, P.; Pande, V.; McCammon, J. A. (2013), Accelerated Molecular Dynamics Simulations with the AMOEBA Polarizable Force Field on Graphics Processing Units. J Chem Theory Comput 9 (11), 4684–4691.

22. Feixas, F.; **Lindert, S.**; Sinko, W.; McCammon, J. A. (2014), Exploring the Role of Receptor Flexibility in Structure-Based Drug Discovery. Biophysical Chemistry 186C, 31-45.

23. **Lindert, S.***; Maslennikov I.*; Chiu E.; Pierce, L.C.; McCammon, J. A.; Choe, S. (2014), Drug screening strategy for human membrane proteins: From NMR protein backbone structure to in silica- and NMR-screened hits. Biochem Biophys Res Commun 445 (4), 724-733.

24. Goetz, A.; Bucher, D.; **Lindert, S.**; McCammon, J. A. (2014), Dipeptide aggregation in aqueous solution from fixed point-charge force fields. J Chem Theory Comput 10 (4), 1631–1637.

25. Liu, Y. L.*; **Lindert, S.***; Zhu, W.; Wang, K.; McCammon, J. A.; Oldfield, E. (2014), Taxodione and arenarone inhibit farnesyl diphosphate synthase by binding to the isopentenyl diphosphate site. Proc Natl Acad Sci U S A 111 (25), E2530-E2539.

26. Rao, V. S.; Cheng, Y.; **Lindert, S.**; Wang, D.; Oxenford, L.; McCulloch, A. D.; McCammon, J. A.; Regnier, M. (2014), PKA phosphorylation of cardiac troponin I modulates activation and relaxation kinetics of ventricular myofibrils. Biophys J 107 (5), 1196-1204.

27. Cheng, Y.; **Lindert, S.**; Kekenes-Huskey, P. M.; Rao, V. S.; Solaro, R.J.; Rosevear, P.R.; Amaro, R.; McCulloch, A. D.; McCammon, J. A.; Regnier, M. (2014), Computational Studies of S23D/S24D Troponin I Mutation on Cardiac Troponin Structural Dynamics. Biophys J. 107 (7), 1675-1685.

28. Zinsser V. L.; **Lindert, S.**; Banford, S.; Hoey, E. M.; Trudgett, A.; Timson, D. J. (2015), UDP-galactose 4'-epimerase from the liver fluke, Fasciola hepatica: biochemical characterisation of the enzyme and identification of inhibitors. Parasitology 142 (3), 463-472.

29. **Lindert, S.**; Li, M. X.; Sykes, B.; McCammon, J.A. (2015), Computer-aided drug discovery approach finds calcium sensitizer of cardiac troponin. Chem Biol Drug Des 85 (2), 99-106.

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.

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.

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.

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.

* signifies equal contribution

SELECTED SCIENTIFIC PRESENTATIONS AND ABSTRACTS:

1. **S. Lindert**, J.A. McCammon. (2014) Differences in troponin C dynamics between cardiac and skeletal muscle – a molecular dynamics perspective. Gordon Research Conference on Biopolymers, abstract, Newport, RI
2. **S. Lindert**, J.A. McCammon. (2014) Differences in troponin C dynamics between cardiac and skeletal muscle – a molecular dynamics perspective. Biophysical Society Annual Meeting, abstract, San Francisco, CA

3. **S. Lindert**, J.A. McCammon. (2013) Molecular Dynamics and calcium binding studies on troponin mutations causing dilated cardiomyopathy. American Heart Association Scientific Sessions, abstract, Dallas, TX

4. **S. Lindert**, J.A. McCammon. (2013) Finding novel anticancer and antibacterial drug leads using CADD - Farnesyl diphosphate synthase (FPPS) and undecaprenyl diphosphate synthase (UPPS) inhibitors from in silico screening. Gordon Research Conference on Computer Aided Drug Design, abstract, Dover, VT

5. **S. Lindert**, J.A. McCammon. (2013) Differences in troponin C dynamics between cardiac and skeletal muscle – a molecular dynamics perspective. Protein Society Annual Meeting, abstract, Boston, MA

6. **S. Lindert**, J.A. McCammon. (2013) Analysis of free energy of opening the Troponin C binding pocket for Troponin I using microsecond molecular dynamics simulations. Biophysical Society Annual Meeting, abstract, Philadelphia, PA

7. **S. Lindert**, J.A. McCammon. (2012) Molecular Dynamics and Calcium Binding Studies on Troponin C. Gordon Research Conference on Computational Chemistry, abstract, Dover, VT

8. **S. Lindert**, P.L. Stewart and J. Meiler. (2010) BCL::EM-Fold: Protein Folding tool for medium resolution density maps. 5th international conference on structural analysis of supramolecular assemblies by hybrid methods, abstract, Lake Tahoe, CA

9. **S. Lindert**, P.L. Stewart and J. Meiler. (2009) BCL::EM-Fit and BCL::EM-Fold: Protein Fitting and Folding tools for medium resolution cryoEM density maps. RosettaCon, abstract, Seattle, WA

10. **S. Lindert**, P.L. Stewart and J. Meiler. (2009) BCL::EM-Fit and BCL::EM-Fold: Protein Fitting and Folding tools for medium resolution cryoEM density maps. Gordon Research Conference on Three Dimensional Electron Microscopy, abstract, New London, NH

11. **S. Lindert**, P.L. Stewart and J. Meiler. (2009). CryoEM guided de novo Protein Fold Elucidation. Biophysical Society Annual Meeting, abstract, Boston, MA

12. **S. Lindert**, P.L. Stewart and J. Meiler. (2008) Building an Atomic Protein Model from a cryoEM Density Map. Keystone Conference on Structural Biology, abstract, Steamboat Springs, CO

13. **S. Lindert**, P.L. Stewart and J. Meiler. (2007) EM-Fold: A Novel Approach for Protein Structure Elucidation from CryoEM Density Maps. Gordon Research Conference on Three Dimensional Electron Microscopy, abstract, New London, NH

PROFESSIONAL ORGANIZATIONS:

2011–present American Heart Association
2011–present American Chemical Society
2011–present Protein Society
2009–present Biophysical Society
2003–present German Physical Society

UNIVERSITY SERVICE:

2009–2011 Vanderbilt University Chemical and Physical Biology Graduate Student Association, Vice President of Academic Affairs

TEACHING EXPERIENCE:

2014 Instructor at Simula Summer School in Computational Physiology, UCSD
2013 Instructor at Membrane Protein Structures by Cell-Free Synthesis, NMR Spectroscopy and Dynamics Workshop, Academia Sinica, Taipei, Taiwan
2013 "Protein Structure Prediction" section of Applied Bioinformatics (CHEM280), Chemistry Department, UCSD
2011, 2012 Instructor at National Biomedical Computational Resource Summer Institute, UCSD
2007 Teaching Assistant for Physical Chemistry, Chemistry Department, Vanderbilt University
2000–2005 Math and Physics tutoring