Steffen Lindert

List of Publications by Year
in descending order

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74 papers	3,377 citations	147801 31 h-index	168389 53 g-index
82 all docs	82 docs citations	82 times ranked	4218 citing authors

#	Article	IF	Citations
1	Protein Structure Prediction with Mass Spectrometry Data. Annual Review of Physical Chemistry, 2022, 73, 1-19.	10.8	18
2	Protein structure prediction using residue-resolved protection factors from hydrogen-deuterium exchange NMR. Structure, 2022, 30, 313-320.e3.	3.3	11
3	Accounting for Neighboring Residue Hydrophobicity in Diethylpyrocarbonate Labeling Mass Spectrometry Improves Rosetta Protein Structure Prediction. Journal of the American Society for Mass Spectrometry, 2022, 33, 584-591.	2.8	8
4	Validated determination of NRG1 Ig-like domain structure by mass spectrometry coupled with computational modeling. Communications Biology, 2022, 5, 452.	4.4	6
5	Simulation of Energy-Resolved Mass Spectrometry Distributions from Surface-Induced Dissociation. Analytical Chemistry, 2022, 94, 10506-10514.	6.5	2
6	Accurate protein structure prediction with hydroxyl radical protein footprinting data. Nature Communications, 2021, 12, 341.	12.8	31
7	Binding of calcium and magnesium to human cardiac troponin C. Journal of Biological Chemistry, 2021, 296, 100350.	3.4	13
8	Identification of Novel Cyclin A2 Binding Site and Nanomolar Inhibitors of Cyclin A2-CDK2 Complex. Current Computer-Aided Drug Design, 2021, 17, 57-68.	1.2	4
9	Protein Structure Prediction from NMR Hydrogenâ€“Deuterium Exchange Data. Journal of Chemical Theory and Computation, 2021, 17, 2619-2629.	5.3	25
10	Prediction of Protein Complex Structure Using Surface-Induced Dissociation and Cryo-Electron Microscopy. Analytical Chemistry, 2021, 93, 7596-7605.	6.5	13
11	Utilization of Hydrophobic Microenvironment Sensitivity in Diethylpyrocarbonate Labeling for Protein Structure Prediction. Analytical Chemistry, 2021, 93, 8188-8195.	6.5	20
12	Adaptative Steered Molecular Dynamics Study of Mutagenesis Effects on Calcium Affinity in the Regulatory Domain of Cardiac Troponin C. Journal of Chemical Information and Modeling, 2021, 61, 3052-3057.	5.4	9
13	Computational Methods Elucidate Consequences of Mutations and Post-translational Modifications on Troponin I Effective Concentration to Troponin C. Journal of Physical Chemistry B, 2021, 125, 7388-7396.	2.6	8
14	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. Journal of Medicinal Chemistry, 2021, 64, 15214-15249.	6.4	16
15	Using NMR Chemical Shifts and Cryo-EM Density Restraints in Iterative Rosetta-MD Protein Structure Refinement. Journal of Chemical Information and Modeling, 2020, 60, 2522-2532.	5.4	19
16	Dioxane-Linked Amide Derivatives as Novel Bacterial Topoisomerase Inhibitors against Gram-Positive Staphylococcus aureus. ACS Medicinal Chemistry Letters, 2020, 11, 2446-2454.	2.8	15
17	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	19.0	513
18	Discovery of Novel Small-Molecule Calcium Sensitizers for Cardiac Troponin C: A Combined Virtual and Experimental Screening Approach. Journal of Chemical Information and Modeling, 2020, 60, 3648-3661.	5.4	25

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19	Hybrid methods for combined experimental and computational determination of protein structure. Journal of Chemical Physics, 2020, 153, 240901.	3.0	48
20	Measuring Intrinsic Disorder and Tracking Conformational Transitions Using Rosetta ResidueDisorder. Journal of Physical Chemistry B, 2019, 123, 7103-7112.	2.6	12
21	Computational Studies of Cardiac and Skeletal Troponin. Frontiers in Molecular Biosciences, 2019, 6, 68.	3.5	18
22	Predicting Protein Complex Structure from Surface-Induced Dissociation Mass Spectrometry Data. ACS Central Science, 2019, 5, 1330-1341.	11.3	37
23	Mechanism of Cardiac Troponin C Calcium Sensitivity Modulation by Small Molecules Illuminated by Umbrella Sampling Simulations. Journal of Chemical Information and Modeling, 2019, 59, 2964-2972.	5.4	11
24	1,3-Dioxane-Linked Bacterial Topoisomerase Inhibitors with Enhanced Antibacterial Activity and Reduced hERG Inhibition. ACS Infectious Diseases, 2019, 5, 1115-1128.	3.8	23
25	Utility of Covalent Labeling Mass Spectrometry Data in Protein Structure Prediction with Rosetta. Journal of Chemical Theory and Computation, 2019, 15, 3410-3424.	5.3	26
26	Relative interfacial cleavage energetics of protein complexes revealed by surface collisions. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 8143-8148.	7.1	60
27	Integrated Use of Biochemical, Native Mass Spectrometry, Computational, and Genome-Editing Methods to Elucidate the Mechanism of a deglycase. Journal of Molecular Biology, 2019, 431, 4497-4513.	4.2	9
28	Improving inverse docking target identification with Zâ€score selection. Chemical Biology and Drug Design, 2019, 93, 1105-1116.	3.2	17
29	Accurately Predicting Disordered Regions of Proteins Using Rosetta ResidueDisorder Application. Journal of Physical Chemistry B, 2018, 122, 3920-3930.	2.6	22
30	Cell-Permeable Bicyclic Peptidyl Inhibitors against NEMO-IÎºB Kinase Interaction Directly from a Combinatorial Library. Journal of the American Chemical Society, 2018, 140, 12102-12110.	13.7	52
31	Molecular Dynamics and Umbrella Sampling Simulations Elucidate Differences in Troponin C Isoform and Mutant Hydrophobic Patch Exposure. Journal of Physical Chemistry B, 2018, 122, 7874-7883.	2.6	21
32	Rosetta Protein Structure Prediction from Hydroxyl Radical Protein Footprinting Mass Spectrometry Data. Analytical Chemistry, 2018, 90, 7721-7729.	6.5	51
33	Iterative Molecular Dynamicsâ€“Rosetta Membrane Protein Structure Refinement Guided by Cryo-EM Densities. Journal of Chemical Theory and Computation, 2017, 13, 5131-5145.	5.3	27
34	Successful Identification of Cardiac Troponin Calcium Sensitizers Using a Combination of Virtual Screening and ROC Analysis of Known Troponin C Binders. Journal of Chemical Information and Modeling, 2017, 57, 3056-3069.	5.4	24
35	The Roles of Actin-Binding Domains 1 and 2 in the Calcium-Dependent Regulation of Actin Filament Bundling by Human Plastins. Journal of Molecular Biology, 2017, 429, 2490-2508.	4.2	37
36	Computational methods in drug discovery. Beilstein Journal of Organic Chemistry, 2016, 12, 2694-2718.	2.2	418

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37	Structures reveal details of small molecule binding to cardiac troponin. Journal of Molecular and Cellular Cardiology, 2016, 101, 134-144.	1.9	39
38	Effects of Cardiac Troponin I Mutation P83S on Contractile Properties and the Modulation by PKA-Mediated Phosphorylation. Journal of Physical Chemistry B, 2016, 120, 8238-8253.	2.6	15
39	Molecular Effects of cTnC DCM Mutations on Calcium Sensitivity and Myofilament Activationâ€"An Integrated Multiscale Modeling Study. Journal of Physical Chemistry B, 2016, 120, 8264-8275.	2.6	18
40	Troponin I Mutations R146G and R21C Alter Cardiac Troponin Function, Contractile Properties, and Modulation by Protein Kinase A (PKA)-mediated Phosphorylation. Journal of Biological Chemistry, 2015, 290, 27749-27766.	3.4	36
41	UDP-galactose 4â€²-epimerase from the liver fluke, Fasciola hepatica: biochemical characterization of the enzyme and identification of inhibitors. Parasitology, 2015, 142, 463-472.	1.5	6
42	Antiinfectives targeting enzymes and the proton motive force. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E7073-82.	7.1	138
43	Computerâ€Aided Drug Discovery Approach Finds Calcium Sensitizer of Cardiac Troponin. Chemical Biology and Drug Design, 2015, 85, 99-106.	3.2	36
44	Improved cryoEM-Guided Iterative Molecular Dynamicsâ€“Rosetta Protein Structure Refinement Protocol for High Precision Protein Structure Prediction. Journal of Chemical Theory and Computation, 2015, 11, 1337-1346.	5.3	33
45	Effects of HCM cTnI Mutation R145G on Troponin Structure and Modulation by PKA Phosphorylation Elucidated by Molecular Dynamics Simulations. Biophysical Journal, 2015, 108, 395-407.	0.5	43
46	A Molecular Dynamics Investigation of Mycobacterium tuberculosis Prenyl Synthases: Conformational Flexibility and Implications for Computerâ€aided Drug Discovery. Chemical Biology and Drug Design, 2015, 85, 756-769.	3.2	14
47	In silico screening for Plasmodium falciparum enoyl-ACP reductase inhibitors. Journal of Computer-Aided Molecular Design, 2015, 29, 79-87.	2.9	18
48	Taxodione and arenarone inhibit farnesyl diphosphate synthase by binding to the isopentenyl diphosphate site. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E2530-9.	7.1	34
49	Exploring the role of receptor flexibility in structure-based drug discovery. Biophysical Chemistry, 2014, 186, 31-45.	2.8	129
50	Computational Studies of the Effect of the S23D/S24D Troponin I Mutation on Cardiac Troponin Structural Dynamics. Biophysical Journal, 2014, 107, 1675-1685.	0.5	48
51	Dipeptide Aggregation in Aqueous Solution from Fixed Point-Charge Force Fields. Journal of Chemical Theory and Computation, 2014, 10, 1631-1637.	5.3	10
52	PKA Phosphorylation of Cardiac Troponin I Modulates Activation andÂRelaxation Kinetics of Ventricular Myofibrils. Biophysical Journal, 2014, 107, 1196-1204.	0.5	45
53	Drug screening strategy for human membrane proteins: From NMR protein backbone structure to in silica- and NMR-screened hits. Biochemical and Biophysical Research Communications, 2014, 445, 724-733.	2.1	11
54	Comparison of dynamics of wildtype and V94M human UDP-galactose 4-epimeraseâ€"A computational perspective on severe epimerase-deficiency galactosemia. Gene, 2013, 526, 318-324.	2.2	17

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55	Iterative Molecular Dynamicsâ€"Rosetta Protein Structure Refinement Protocol to Improve Model Quality. Journal of Chemical Theory and Computation, 2013, 9, 3843-3847.	5.3	39
56	AutoGrow 3.0: An improved algorithm for chemically tractable, semi-automated protein inhibitor design. Journal of Molecular Graphics and Modelling, 2013, 44, 104-112.	2.4	48
57	Computational determination of the orientation of a heat repeat-like domain of DNA-PKcs. Computational Biology and Chemistry, 2013, 42, 1-4.	2.3	1
58	Accelerated Molecular Dynamics Simulations with the AMOEBA Polarizable Force Field on Graphics Processing Units. Journal of Chemical Theory and Computation, 2013, 9, 4684-4691.	5.3	39
59	Farnesyl Diphosphate Synthase Inhibitors from In Silico Screening. Chemical Biology and Drug Design, 2013, 81, 742-748.	3.2	42
60	Accounting for Receptor Flexibility and Enhanced Sampling Methods in Computerâ€Aided Drug Design. Chemical Biology and Drug Design, 2013, 81, 41-49.	3.2	100
61	Antibacterial drug leads targeting isoprenoid biosynthesis. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 123-128.	7.1	129
62	Molecular Basis of Calcium-Sensitizing and Desensitizing Mutations of the Human Cardiac Troponin C Regulatory Domain: A Multi-Scale Simulation Study. PLoS Computational Biology, 2012, 8, e1002777.	3.2	36
63	Dynamics of Plasmodium falciparum enoylâ€ACP reductase and implications on drug discovery. Protein Science, 2012, 21, 1734-1745.	7.6	9
64	Dynamics and Calcium Association to the N-Terminal Regulatory Domain of Human Cardiac Troponin C: A Multiscale Computational Study. Journal of Physical Chemistry B, 2012, 116, 8449-8459.	2.6	46
65	Long-Timescale Molecular Dynamics Simulations Elucidate the Dynamics and Kinetics of Exposure of the Hydrophobic Patch in Troponin C. Biophysical Journal, 2012, 103, 1784-1789.	0.5	39
66	LigMerge: A Fast Algorithm to Generate Models of Novel Potential Ligands from Sets of Known Binders. Chemical Biology and Drug Design, 2012, 80, 358-365.	3.2	17
67	EM-Fold: De Novo Atomic-Detail Protein Structure Determination from Medium-Resolution Density Maps. Structure, 2012, 20, 464-478.	3.3	86
68	Ab initio protein modeling into CryoEM density maps using EMâ€Fold. Biopolymers, 2012, 97, 669-677.	2.4	23
69	BCL::EM-Fit: Rigid body fitting of atomic structures into density maps using geometric hashing and real space refinement. Journal of Structural Biology, 2011, 175, 264-276.	2.8	33
70	Insight into the Mechanisms of Adenovirus Capsid Disassembly from Studies of Defensin Neutralization. PLoS Pathogens, 2010, 6, e1000959.	4.7	109
71	Cryo-Electron Microscopy Structure of an Adenovirus-Integrin Complex Indicates Conformational Changes in both Penton Base and Integrin. Journal of Virology, 2009, 83, 11491-11501.	3.4	53
72	Cryo-Electron Microscopy Structure of Adenovirus Type 2 Temperature-Sensitive Mutant 1 Reveals Insight into the Cell Entry Defect. Journal of Virology, 2009, 83, 7375-7383.	3.4	48

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73	Hybrid approaches: applying computational methods in cryo-electron microscopy. Current Opinion in Structural Biology, 2009, 19, 218-225.	5.7	37
74	EM-Fold: De Novo Folding of Î±-Helical Proteins Guided by Intermediate-Resolution Electron Microscopy Density Maps. Structure, 2009, 17, 990-1003.	3.3	76