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	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	19.0	513
2	Computational methods in drug discovery. Beilstein Journal of Organic Chemistry, 2016, 12, 2694-2718.	2.2	418
3	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
4	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
5	Exploring the role of receptor flexibility in structure-based drug discovery. Biophysical Chemistry, 2014, 186, 31-45.	2.8	129
6	Insight into the Mechanisms of Adenovirus Capsid Disassembly from Studies of Defensin Neutralization. PLoS Pathogens, 2010, 6, e1000959.	4.7	109
7	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
8	EM-Fold: De Novo Atomic-Detail Protein Structure Determination from Medium-Resolution Density Maps. Structure, 2012, 20, 464-478.	3.3	86
9	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
10	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
11	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
12	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
13	Rosetta Protein Structure Prediction from Hydroxyl Radical Protein Footprinting Mass Spectrometry Data. Analytical Chemistry, 2018, 90, 7721-7729.	6.5	51
14	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
15	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
16	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
17	Hybrid methods for combined experimental and computational determination of protein structure. Journal of Chemical Physics, 2020, 153, 240901.	3.0	48
18	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

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19	PKA Phosphorylation of Cardiac Troponin I Modulates Activation andÂRelaxation Kinetics of Ventricular Myofibrils. Biophysical Journal, 2014, 107, 1196-1204.	0.5	45
20	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
21	Farnesyl Diphosphate Synthase Inhibitors from In Silico Screening. Chemical Biology and Drug Design, 2013, 81, 742-748.	3.2	42
22	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
23	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
24	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
25	Structures reveal details of small molecule binding to cardiac troponin. Journal of Molecular and Cellular Cardiology, 2016, 101, 134-144.	1.9	39
26	Hybrid approaches: applying computational methods in cryo-electron microscopy. Current Opinion in Structural Biology, 2009, 19, 218-225.	5.7	37
27	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
28	Predicting Protein Complex Structure from Surface-Induced Dissociation Mass Spectrometry Data. ACS Central Science, 2019, 5, 1330-1341.	11.3	37
29	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
30	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
31	Computerâ€Aided Drug Discovery Approach Finds Calcium Sensitizer of Cardiac Troponin. Chemical Biology and Drug Design, 2015, 85, 99-106.	3.2	36
32	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
33	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
34	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
35	Accurate protein structure prediction with hydroxyl radical protein footprinting data. Nature Communications, 2021, 12, 341.	12.8	31
36	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

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37	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
38	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
39	Protein Structure Prediction from NMR Hydrogenâ€“Deuterium Exchange Data. Journal of Chemical Theory and Computation, 2021, 17, 2619-2629.	5.3	25
40	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
41	Ab initio protein modeling into CryoEM density maps using EMâ€Fold. Biopolymers, 2012, 97, 669-677.	2.4	23
42	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
43	Accurately Predicting Disordered Regions of Proteins Using Rosetta ResidueDisorder Application. Journal of Physical Chemistry B, 2018, 122, 3920-3930.	2.6	22
44	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
45	Utilization of Hydrophobic Microenvironment Sensitivity in Diethylpyrocarbonate Labeling for Protein Structure Prediction. Analytical Chemistry, 2021, 93, 8188-8195.	6.5	20
46	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
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	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
49	Computational Studies of Cardiac and Skeletal Troponin. Frontiers in Molecular Biosciences, 2019, 6, 68.	3.5	18
50	Protein Structure Prediction with Mass Spectrometry Data. Annual Review of Physical Chemistry, 2022, 73, 1-19.	10.8	18
51	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
52	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
53	Improving inverse docking target identification with Zâ€score selection. Chemical Biology and Drug Design, 2019, 93, 1105-1116.	3.2	17
54	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

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55	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
56	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
57	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
58	Binding of calcium and magnesium to human cardiac troponin C. Journal of Biological Chemistry, 2021, 296, 100350.	3.4	13
59	Prediction of Protein Complex Structure Using Surface-Induced Dissociation and Cryo-Electron Microscopy. Analytical Chemistry, 2021, 93, 7596-7605.	6.5	13
60	Measuring Intrinsic Disorder and Tracking Conformational Transitions Using Rosetta ResidueDisorder. Journal of Physical Chemistry B, 2019, 123, 7103-7112.	2.6	12
61	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
62	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
63	Protein structure prediction using residue-resolved protection factors from hydrogen-deuterium exchange NMR. Structure, 2022, 30, 313-320.e3.	3.3	11
64	Dipeptide Aggregation in Aqueous Solution from Fixed Point-Charge Force Fields. Journal of Chemical Theory and Computation, 2014, 10, 1631-1637.	5.3	10
65	Dynamics of Plasmodium falciparum enoylâ€ACP reductase and implications on drug discovery. Protein Science, 2012, 21, 1734-1745.	7.6	9
66	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
67	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
68	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
69	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
70	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
71	Validated determination of NRG1 Ig-like domain structure by mass spectrometry coupled with computational modeling. Communications Biology, 2022, 5, 452.	4.4	6
72	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

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73	Simulation of Energy-Resolved Mass Spectrometry Distributions from Surface-Induced Dissociation. Analytical Chemistry, 2022, 94, 10506-10514.	6.5	2
74	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