Erik R Lindahl

List of Publications by Year
in descending order

130	69,315	39113 52	16186 128
papers	citations	h-index	g-index

154	154	154	65394
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	<scp>Preâ€exascale HPC</scp> approaches for molecular dynamics simulations. Covidâ€19 research: A use case. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	6
2	Structures of highly flexible intracellular domain of human Î±7 nicotinic acetylcholine receptor. Nature Communications, 2022, 13, 793.	5.8	23
3	Probing effects of the SARS-CoV-2 E protein on membrane curvature and intracellular calcium. Biochimica Et Biophysica Acta - Biomembranes, 2022, 1864, 183994.	1.4	11
4	Allosteric enhancement of the BCR-Abl1 kinase inhibition activity of nilotinib by cobinding of asciminib. Journal of Biological Chemistry, 2022, 298, 102238.	1.6	13
5	Molecular Reorganization during the Formation of the Human Skin Barrier Studied In Situ. Journal of Investigative Dermatology, 2021, 141, 1243-1253.e6.	0.3	16
6	Bacterial protein domains with a novel Igâ€like fold target human CEACAM receptors. EMBO Journal, 2021, 40, e106103.	3.5	16
7	A Blueprint for High Affinity SARS-CoV-2 Mpro Inhibitors from Activity-Based Compound Library Screening Guided by Analysis of Protein Dynamics. ACS Pharmacology and Translational Science, 2021, 4, 1079-1095.	2.5	44
8	Dynamic closed states of a ligand-gated ion channel captured by cryo-EM and simulations. Life Science Alliance, 2021, 4, e202101011.	1.3	16
9	Regulation of a pentameric ligand-gated ion channel by a semiconserved cationic lipid-binding site. Journal of Biological Chemistry, 2021, 297, 100899.	1.6	15
10	Probing solution structure of the pentameric ligand-gated ion channel GLIC by small-angle neutron scattering. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	7
11	Markov state models of proton- and pore-dependent activation in a pentameric ligand-gated ion channel. ELife, 2021, 10, .	2.8	9
12	Computational Studies of SARS-CoV-2 3CLpro: Insights from MD Simulations. International Journal of Molecular Sciences, 2020, 21, 5346.	1.8	48
13	Heterogeneous parallelization and acceleration of molecular dynamics simulations in GROMACS. Journal of Chemical Physics, 2020, 153, 134110.	1.2	275
14	Shared structural mechanisms of general anaesthetics and benzodiazepines. Nature, 2020, 585, 303-308.	13.7	195
15	Structural basis for allosteric transitions of a multidomain pentameric ligand-gated ion channel. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 13437-13446.	3.3	18
16	Structural basis for the increased processivity of D-family DNA polymerases in complex with PCNA. Nature Communications, 2020, 11, 1591.	5.8	34
17	An angular motion of a conserved four-helix bundle facilitates alternating access transport in the TtNapA and EcNhaA transporters. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 31850-31860.	3.3	6
18	Development of basic building blocks for cryo-EM: the emcore and emvis software libraries. Acta Crystallographica Section D: Structural Biology, 2020, 76, 350-356.	1.1	0

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19	Agonist Selectivity and Ion Permeation in the Î±3Î²4 Ganglionic Nicotinic Receptor. Neuron, 2019, 104, 501-511.e6.	3.8	131
20	Sharing Data from Molecular Simulations. Journal of Chemical Information and Modeling, 2019, 59, 4093-4099.	2.5	26
21	Structure of the DP1â€“DP2 PolD complex bound with DNA and its implications for the evolutionary history of DNA and RNA polymerases. PLoS Biology, 2019, 17, e3000122.	2.6	30
22	Ten simple rules on how to create open access and reproducible molecular simulations of biological systems. PLoS Computational Biology, 2019, 15, e1006649.	1.5	25
23	Structure of the human ClC-1 chloride channel. PLoS Biology, 2019, 17, e3000218.	2.6	66
24	eBDIMS server: protein transition pathways with ensemble analysis in 2D-motion spaces. Bioinformatics, 2019, 35, 3505-3507.	1.8	19
25	Inhibition of Nuclear PTEN Tyrosine Phosphorylation Enhances Glioma Radiation Sensitivity through Attenuated DNA Repair. Cancer Cell, 2019, 35, 504-518.e7.	7.7	102
26	The Future of Swedish e-Science: SeRC 2.0. , 2019, , .		0
27	Doping of metastable Cu3N at different Ni concentrations: Growth, crystallographic sites and resistivity. Thin Solid Films, 2018, 647, 1-8.	0.8	6
28	Structural Basis for a Bimodal Allosteric Mechanism of General Anesthetic Modulation in Pentameric Ligand-Gated Ion Channels. Cell Reports, 2018, 23, 993-1004.	2.9	33
29	Human skin barrier structure and function analyzed by cryo-EM and molecular dynamics simulation. Journal of Structural Biology, 2018, 203, 149-161.	1.3	57
30	Structure of the chloroplast ribosome with chl-RRF and hibernation-promoting factor. Nature Plants, 2018, 4, 212-217.	4.7	61
31	Structural Transitions in Ceramide Cubic Phases during Formation of the Human Skin Barrier. Biophysical Journal, 2018, 114, 1116-1127.	0.2	13
32	e-Science in Scandinavia. Informatik-Spektrum, 2018, 41, 398-404.	1.0	1
33	Allosteric potentiation of a ligand-gated ion channel is mediated by access to a deep membrane-facing cavity. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10672-10677.	3.3	31
34	Determining the molecular basis of voltage sensitivity in membrane proteins. Journal of General Physiology, 2018, 150, 1444-1458.	0.9	16
35	Predicting drug permeability through skin using molecular dynamics simulation. Journal of Controlled Release, 2018, 283, 269-279.	4.8	90
36	Characterisation of molecular motions in cryo-EM single-particle data by multi-body refinement in RELION. ELife, 2018, 7, .	2.8	434

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37	New tools for automated high-resolution cryo-EM structure determination in RELION-3. ELife, 2018, 7, .	2.8	3,965
38	A drug pocket at the lipid bilayerâ€“potassium channel interface. Science Advances, 2017, 3, e1701099.	4.7	19
39	Cryo-EM reconstruction of the chlororibosome to 3.2â€…Ã… resolution within 24â€…h. IUCrJ, 2017, 4, 723-727.	1.0	3
40	Accelerated cryo-EM structure determination with parallelisation using GPUs in RELION-2. ELife, 2016, 5, .	2.8	919
41	Functional characterization of neurotransmitter activation and modulation in a nematode model ligandâ€gated ion channel. Journal of Neurochemistry, 2016, 138, 243-253.	2.1	5
42	Reciprocal voltage sensor-to-pore coupling leads to potassium channel C-type inactivation. Scientific Reports, 2016, 6, 27562.	1.6	18
43	Membrane Anchoring and Ion-Entry Dynamics in P-type ATPase Copper Transport. Biophysical Journal, 2016, 111, 2417-2429.	0.2	16
44	Allosteric binding site in a Cys-loop receptor ligand-binding domain unveiled in the crystal structure of ELIC in complex with chlorpromazine. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E6696-E6703.	3.3	30
45	Prediction and validation of protein intermediate states from structurally rich ensembles and coarse-grained simulations. Nature Communications, 2016, 7, 12575.	5.8	62
46	Energetics of side-chain snorkeling in transmembrane helices probed by nonproteinogenic amino acids. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 10559-10564.	3.3	26
47	The Molecular Basis of Polyunsaturated Fatty Acid Interactions with the Shaker Voltage-Gated Potassium Channel. PLoS Computational Biology, 2016, 12, e1004704.	1.5	47
48	Conformational Gating Dynamics in the GluCl Anion-Selective Chloride Channel. ACS Chemical Neuroscience, 2015, 6, 1459-1467.	1.7	18
49	Tackling Exascale Software Challenges in Molecular Dynamics Simulations with GROMACS. Lecture Notes in Computer Science, 2015, , 3-27.	1.0	581
50	Coupled Diffusion in Lipid Bilayers upon Close Approach. Journal of the American Chemical Society, 2015, 137, 708-714.	6.6	14
51	GROMACS: High performance molecular simulations through multi-level parallelism from laptops to supercomputers. SoftwareX, 2015, 1-2, 19-25.	1.2	14,414
52	SAXS-Guided Metadynamics. Journal of Chemical Theory and Computation, 2015, 11, 3491-3498.	2.3	37
53	Molecular Simulation Workflows as Parallel Algorithms: The Execution Engine of Copernicus, a Distributed High-Performance Computing Platform. Journal of Chemical Theory and Computation, 2015, 11, 2600-2608.	2.3	40
54	Direct-Space Corrections Enable Fast and Accurate Lorentzâ€“Berthelot Combination Rule Lennard-Jones Lattice Summation. Journal of Chemical Theory and Computation, 2015, 11, 5737-5746.	2.3	112

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55	Automatic GROMACS Topology Generation and Comparisons of Force Fields for Solvation Free Energy Calculations. Journal of Physical Chemistry B, 2015, 119, 810-823.	1.2	88
56	Molecular Dynamics Simulations. Methods in Molecular Biology, 2015, 1215, 3-26.	0.4	41
57	An efficient and extensible format, library, and API for binary trajectory data from molecular simulations. Journal of Computational Chemistry, 2014, 35, 260-269.	1.5	14
58	Structural Models of Ligandâ€Gated Ion Channels: Sites of Action for Anesthetics and Ethanol. Alcoholism: Clinical and Experimental Research, 2014, 38, 595-603.	1.4	47
59	Dynamic heterogeneity controls diffusion and viscosity near biological interfaces. Nature Communications, 2014, 5, 3034.	5.8	58
60	From Side Chains Rattling on Picoseconds to Ensemble Simulations of Protein Folding. Israel Journal of Chemistry, 2014, 54, 1274-1285.	1.0	0
61	Preparing Scientific Application Software for Exascale Computing. Lecture Notes in Computer Science, 2013, , 27-42.	1.0	4
62	The C-terminal cavity of the Na,K-ATPase analyzed by docking and electrophysiology. Molecular Membrane Biology, 2013, 30, 195-205.	2.0	7
63	The Conserved Phenylalanine in the K+ Channel Voltage-Sensor Domain Creates a Barrier with Unidirectional Effects. Biophysical Journal, 2013, 104, 75-84.	0.2	21
64	A specific interdomain interaction preserves the structural and binding properties of the ModA protein from the phytopathogen Xanthomonas citri domain interaction and transport in ModA. Archives of Biochemistry and Biophysics, 2013, 539, 20-30.	1.4	3
65	Functional Validation of Virtual Screening for Novel Agents with General Anesthetic Action at Ligand-Gated Ion Channels. Molecular Pharmacology, 2013, 84, 670-678.	1.0	19
66	Lennard-Jones Lattice Summation in Bilayer Simulations Has Critical Effects on Surface Tension and Lipid Properties. Journal of Chemical Theory and Computation, 2013, 9, 3527-3537.	2.3	138
67	Probing microscopic material properties inside simulated membranes through spatially resolved three-dimensional local pressure fields and surface tensions. Chemistry and Physics of Lipids, 2013, 169, 106-112.	1.5	11
68	Stabilization of the GluCl Ligand-Gated Ion Channel in the Presence andÂAbsence of Ivermectin. Biophysical Journal, 2013, 105, 640-647.	0.2	26
69	Inhibition versus Potentiation of Ligand-Gated Ion Channels Can Be Altered by a Single Mutation that Moves Ligands between Intra- and Intersubunit Sites. Structure, 2013, 21, 1307-1316.	1.6	20
70	GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. Bioinformatics, 2013, 29, 845-854.	1.8	6,072
71	Association Dynamics and Linear and Nonlinear Optical Properties of an N-Acetylaladanamide Probe in a POPC Membrane. Journal of the American Chemical Society, 2013, 135, 13590-13597.	6.6	27
72	Assessment of Homology Templates and an Anesthetic Binding Site within the Î³-Aminobutyric Acid Receptor. Anesthesiology, 2013, 119, 1087-1095.	1.3	33

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73	Molecular Mechanism for the Dual Alcohol Modulation of Cys-loop Receptors. PLoS Computational Biology, 2012, 8, e1002710.	1.5	35
74	An emerging consensus on voltage-dependent gating from computational modeling and molecular dynamics simulations. Journal of General Physiology, 2012, 140, 587-594.	0.9	179
75	Unraveling the strokes of ion channel molecular machines in computers. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 21186-21187.	3.3	1
76	Molecular recognition of a single sphingolipid species by a proteinâ€™s transmembrane domain. Nature, 2012, 481, 525-529.	13.7	330
77	Improved model quality assessment using ProQ2. BMC Bioinformatics, 2012, 13, 224.	1.2	173
78	The Free Energy Barrier for Arginine Gating Charge Translation Is Altered by Mutations in the Voltage Sensor Domain. PLoS ONE, 2012, 7, e45880.	1.1	19
79	Tracking a complete voltage-sensor cycle with metal-ion bridges. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 8552-8557.	3.3	132
80	Identification of Selective Inhibitors of the Potassium Channel Kv1.1â€“1.2₍₃₎ by Highâ€Throughput Virtual Screening and Automated Patch Clamp. ChemMedChem, 2012, 7, 1775-1783.	1.6	20
81	Gasâ€Pulsed CVD for Film Growth in the Cuï¿Nïï¿N System. Chemical Vapor Deposition, 2012, 18, 10-16.	1.4	7
82	Structural basis for alcohol modulation of a pentameric ligand-gated ion channel. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 12149-12154.	3.3	102
83	Water Ordering at Membrane Interfaces Controls Fusion Dynamics. Journal of the American Chemical Society, 2011, 133, 3812-3815.	6.6	47
84	310-Helix Conformation Facilitates the Transition of a Voltage Sensor S4 Segment toward the Down State. Biophysical Journal, 2011, 100, 1446-1454.	0.2	54
85	Microsecond Simulations Indicate that Ethanol Binds between Subunits and Could Stabilize an Open-State Model of a Glycine Receptor. Biophysical Journal, 2011, 100, 1642-1650.	0.2	72
86	Algorithm improvements for molecular dynamics simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 93-108.	6.2	30
87	Copernicus. , 2011, , .		27
88	A highâ€performance parallelâ€generalized born implementation enabled by tabulated interaction rescaling. Journal of Computational Chemistry, 2010, 31, 2593-2600.	1.5	20
89	Internal duplications in Î±â€helical membrane protein topologies are common but the nonduplicated forms are rare. Protein Science, 2010, 19, 2305-2318.	3.1	17
90	Model quality assessment for membrane proteins. Bioinformatics, 2010, 26, 3067-3074.	1.8	71

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91	Atomic-Resolution Simulations Predict a Transition State for Vesicle Fusion Defined by Contact of a Few Lipid Tails. PLoS Computational Biology, 2010, 6, e1000829.	1.5	108
92	Normal Mode Gating Motions of a Ligand-Gated Ion Channel Persist in a Fully Hydrated Lipid Bilayer Model. ACS Chemical Neuroscience, 2010, 1, 552-558.	1.7	7
93	Modeling Anesthetic Binding Sites within the Glycine Alpha One Receptor Based on Prokaryotic Ion Channel Templates: The Problem with TM4. Journal of Chemical Information and Modeling, 2010, 50, 2248-2255.	2.5	24
94	Implementation of the CHARMM Force Field in GROMACS: Analysis of Protein Stability Effects from Correction Maps, Virtual Interaction Sites, and Water Models. Journal of Chemical Theory and Computation, 2010, 6, 459-466.	2.3	866
95	Membrane Proteins Diffuse as Dynamic Complexes with Lipids. Journal of the American Chemical Society, 2010, 132, 7574-7575.	6.6	157
96	Conformational Changes and Slow Dynamics through Microsecond Polarized Atomistic Molecular Simulation of an Integral Kv1.2 Ion Channel. PLoS Computational Biology, 2009, 5, e1000289.	1.5	108
97	Chemical Vapour Deposition of Metastable Ni₃N. ECS Transactions, 2009, 25, 365-372.	0.3	10
98	Protein contents in biological membranes can explain abnormal solvation of charged and polar residues. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15684-15689.	3.3	63
99	Titratable Amino Acid Solvation in Lipid Membranes as a Function of Protonation State. Journal of Physical Chemistry B, 2009, 113, 245-253.	1.2	35
100	The role of lipid composition for insertion and stabilization of amino acids in membranes. Journal of Chemical Physics, 2009, 130, 185101.	1.2	61
101	3D Pressure Field in Lipid Membranes and Membrane-Protein Complexes. Physical Review Letters, 2009, 102, 078101.	2.9	180
102	Positionâ€resolved free energy of solvation for amino acids in lipid membranes from molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1332-1344.	1.5	66
103	GROMACS 4:â€‰ Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation. Journal of Chemical Theory and Computation, 2008, 4, 435-447.	2.3	13,875
104	Using multiple templates to improve quality of homology models in automated homology modeling. Protein Science, 2008, 17, 990-1002.	3.1	130
105	Membrane proteins: molecular dynamics simulations. Current Opinion in Structural Biology, 2008, 18, 425-431.	2.6	297
106	Molecular Dynamics Simulations. Methods in Molecular Biology, 2008, 443, 3-23.	0.4	51
107	Effect of Cobratoxin Binding on the Normal Mode Vibration within Acetylcholine Binding Protein. Journal of Chemical Information and Modeling, 2008, 48, 855-860.	2.5	14
108	Prediction of membrane-protein topology from first principles. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 7177-7181.	3.3	288

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109	Normal-Mode Analysis of the Glycine Alpha1 Receptor by Three Separate Methods. Journal of Chemical Information and Modeling, 2007, 47, 1572-1579.	2.5	32
110	Speeding up parallel GROMACS on high-latency networks. Journal of Computational Chemistry, 2007, 28, 2075-2084.	1.5	107
111	Amino-Acid Solvation Structure in Transmembrane Helices from Molecular Dynamics Simulations. Biophysical Journal, 2006, 91, 4450-4463.	0.2	71
112	PDB_Hydro: incorporating dipolar solvents with variable density in the Poisson-Boltzmann treatment of macromolecule electrostatics. Nucleic Acids Research, 2006, 34, W38-W42.	6.5	62
113	NOMAD-Ref: visualization, deformation and refinement of macromolecular structures based on all-atom normal mode analysis. Nucleic Acids Research, 2006, 34, W52-W56.	6.5	292
114	Improved GROMACS Scaling on Ethernet Switched Clusters. Lecture Notes in Computer Science, 2006, , 404-405.	1.0	2
115	GROMACS: Fast, flexible, and free. Journal of Computational Chemistry, 2005, 26, 1701-1718.	1.5	13,676
116	Refinement of docked protein-ligand and protein-DNA structures using low frequency normal mode amplitude optimization. Nucleic Acids Research, 2005, 33, 4496-4506.	6.5	62
117	Normal mode analysis reveals the channel gating motion within a ligand gated ion channel model. International Congress Series, 2005, 1283, 160-163.	0.2	5
118	Simulations of the role of water in the protein-folding mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 6456-6461.	3.3	187
119	Brute-Force Molecular Dynamics Simulations of Villin Headpiece:Â Comparison with NMR Parameters. Journal of Physical Chemistry B, 2003, 107, 11178-11187.	1.2	62
120	Structure and Dynamics of Interfacial Water in an LÎ± Phase Lipid Bilayer from Molecular Dynamics Simulations. Biophysical Journal, 2003, 84, 102-115.	0.2	97
121	Molecular Dynamics Simulations of Phospholipid Bilayers with Cholesterol. Biophysical Journal, 2003, 84, 2192-2206.	0.2	452
122	Molecular dynamics simulation of NMR relaxation rates and slow dynamics in lipid bilayers. Journal of Chemical Physics, 2001, 115, 4938-4950.	1.2	109
123	A direct simulation of EPR slow-motion spectra of spin labelled phospholipids in liquid crystalline bilayers based on a molecular dynamics simulation of the lipid dynamics. Physical Chemistry Chemical Physics, 2001, 3, 5311-5319.	1.3	41
124	Simulation of the Spontaneous Aggregation of Phospholipids into Bilayers. Journal of the American Chemical Society, 2001, 123, 8638-8639.	6.6	242
125	GROMACS 3.0: a package for molecular simulation and trajectory analysis. Journal of Molecular Modeling, 2001, 7, 306-317.	0.8	6,085
126	Isolated Hypervariable Regions Derived from Streptococcal M Proteins Specifically Bind Human C4b-Binding Protein: Implications for Antigenic Variation. Journal of Immunology, 2001, 167, 3870-3877.	0.4	62

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127	Identification of related proteins on family, superfamily and fold level 1 1Edited by F. C. Cohen. Journal of Molecular Biology, 2000, 295, 613-625.	2.0	179
128	Mesoscopic Undulations and Thickness Fluctuations in Lipid Bilayers from Molecular Dynamics Simulations. Biophysical Journal, 2000, 79, 426-433.	0.2	562
129	Spatial and energetic-entropic decomposition of surface tension in lipid bilayers from molecular dynamics simulations. Journal of Chemical Physics, 2000, 113, 3882-3893.	1.2	229
130	Solvent diffusion outside macromolecular surfaces. Physical Review E, 1998, 57, 791-796.	0.8	16