Helgi I IngÃ³lfsson

List of Publications by Year
in descending order

88 papers	6,913 citations	156536 32 h-index	120465 65 g-index
91 all docs	91 docs citations	91 times ranked	7465 citing authors

#	Article	IF	Citations
1	Machine learningâ€“driven multiscale modeling reveals lipid-dependent dynamics of RAS signaling proteins. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	44
2	Regulation of Gramicidin Channel Function Solely by Changes in Lipid Intrinsic Curvature. Frontiers in Physiology, 2022, 13, 836789.	1.3	4
3	Exploring CRD mobility during RAS/RAF engagement at the membrane. Biophysical Journal, 2022, 121, 3630-3650.	0.2	9
4	Machine-learning-based dynamic-importance sampling for adaptive multiscale simulations. Nature Machine Intelligence, 2021, 3, 401-409.	8.3	22
5	Atomistic Characterization of Gramicidin Channel Formation. Journal of Chemical Theory and Computation, 2021, 17, 7-12.	2.3	12
6	Generalizable coordination of large multiscale workflows. , 2021, , .		17
7	Simulations of Asymmetric Membranes Illustrate Cooperative Leaflet Coupling and Lipid Adaptability. Frontiers in Cell and Developmental Biology, 2020, 8, 575.	1.8	26
8	ddcMD: A fully GPU-accelerated molecular dynamics program for the Martini force field. Journal of Chemical Physics, 2020, 153, 045103.	1.2	18
9	Assessing the Perturbing Effects of Drugs on Lipid Bilayers Using Gramicidin Channel-Based In Silico and In Vitro Assays. Journal of Medicinal Chemistry, 2020, 63, 11809-11818.	2.9	10
10	Predicting Small Molecule Transfer Free Energies by Combining Molecular Dynamics Simulations and Deep Learning. Journal of Chemical Information and Modeling, 2020, 60, 5375-5381.	2.5	35
11	Capturing Biologically Complex Tissue-Specific Membranes at Different Levels of Compositional Complexity. Journal of Physical Chemistry B, 2020, 124, 7819-7829.	1.2	47
12	Decoupling copolymer, lipid and carbon nanotube interactions in hybrid, biomimetic vesicles. Nanoscale, 2020, 12, 6545-6555.	2.8	5
13	Using Machine Learning to Predict Membrane Protein States Based on their Lipid Environment. Biophysical Journal, 2020, 118, 497a.	0.2	0
14	Molecular Process of Gramicidin a Dimerization Determined with Milliseconds Atomistic Simulations and Machine Learning. Biophysical Journal, 2020, 118, 555a.	0.2	0
15	Flux: Overcoming scheduling challenges for exascale workflows. Future Generation Computer Systems, 2020, 110, 202-213.	4.9	37
16	A molecular view on the escape of lipoplexed DNA from the endosome. ELife, 2020, 9, .	2.8	46
17	Bridging the Scales: A Machine Learning Directed Macro to Micro Scale Simulation to Model RAS Initiation of Cancer. Biophysical Journal, 2019, 116, 304a.	0.2	0
18	Molecular Mechanism for Gramicidin Dimerization and Dissociation in Bilayers of Different Thickness. Biophysical Journal, 2019, 117, 1831-1844.	0.2	15

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19	MemSurfer: A Tool for Robust Computation and Characterization of Curved Membranes. Journal of Chemical Theory and Computation, 2019, 15, 6411-6421.	2.3	36
20	Multiscale Modeling and Simulation Approaches to Lipidâ€“Protein Interactions. Methods in Molecular Biology, 2019, 2003, 1-30.	0.4	7
21	Memsurfer: A Tool for Robust Computation and Characterization of Bilayer Membranes. Biophysical Journal, 2019, 116, 91a.	0.2	0
22	The Influence of Periodic Size Effects and Membrane Undulation on Phase Separation in a DPPC/DOPC/Chol Coarse Grain Martini System. Biophysical Journal, 2019, 116, 225a.	0.2	0
23	Comparing GPU Power and Frequency Capping: A Case Study with the MuMMI Workflow. , 2019, , .		9
24	Computational Modeling of Realistic Cell Membranes. Chemical Reviews, 2019, 119, 6184-6226.	23.0	502
25	A massively parallel infrastructure for adaptive multiscale simulations. , 2019, , .		32
26	Synthetic Analogues of the Snail Toxin 6-Bromo-2-mercaptotryptamine Dimer (BrMT) Reveal That Lipid Bilayer Perturbation Does Not Underlie Its Modulation of Voltage-Gated Potassium Channels. Biochemistry, 2018, 57, 2733-2743.	1.2	18
27	Martini Coarse-Grained Force Field for RNA. Biophysical Journal, 2018, 114, 437a.	0.2	3
28	Lipid Organization in Simulations of Cell Membranes. Biophysical Journal, 2018, 114, 379a.	0.2	0
29	Lipid composition dictates serum stability of reconstituted high-density lipoproteins: implications for in vivo applications. Nanoscale, 2018, 10, 7420-7430.	2.8	12
30	Complex Biological Membranes: Capturing Bilayer Properties In Silico at Different Compositional Complexity. Biophysical Journal, 2018, 114, 270a.	0.2	0
31	Capturing Phase Behavior of Ternary Lipid Mixtures with a Refined Martini Coarse-Grained Force Field. Journal of Chemical Theory and Computation, 2018, 14, 6050-6062.	2.3	63
32	Folding and Lipid Composition Determine Membrane Interaction of the Disordered Protein COR15A. Biophysical Journal, 2018, 115, 968-980.	0.2	21
33	Cholesterol Flip-Flop Impacts Domain Registration in Plasma Membrane Models. Journal of Physical Chemistry Letters, 2018, 9, 5527-5533.	2.1	36
34	Fluorinated Alcoholsâ€™ Effects on Lipid Bilayer Properties. Biophysical Journal, 2018, 115, 679-689.	0.2	23
35	Accurate Phase Separation of Complex Lipid Mixtures (DPPC/DOPC/CHOL) with a Refined Coarse Grained Martini Model. Biophysical Journal, 2018, 114, 102a.	0.2	0
36	Lipidâ€“Protein Interactions Are Unique Fingerprints for Membrane Proteins. ACS Central Science, 2018, 4, 709-717.	5.3	274

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37	Curvatureâ€Induced Sorting of Lipids in Plasma Membrane Tethers. Advanced Theory and Simulations, 2018, 1, 1800034.	1.3	54
38	High-Throughput Simulations Reveal Membrane-Mediated Effects of Alcohols on MscL Gating. Journal of the American Chemical Society, 2017, 139, 2664-2671.	6.6	41
39	Curvature-Induced Lipid Sorting in Plasma Membrane Tethers. Biophysical Journal, 2017, 112, 467a.	0.2	0
40	Modeling Tissue Specific Plasma Membranes in Silico. Biophysical Journal, 2017, 112, 376a.	0.2	0
41	Martini Coarse-Grained Force Field: Extension to RNA. Biophysical Journal, 2017, 113, 246-256.	0.2	156
42	Lipid and Peptide Diffusion in Bilayers: The Saffmanâ€“DelbrÃ¼ck Model and Periodic Boundary Conditions. Journal of Physical Chemistry B, 2017, 121, 3443-3457.	1.2	91
43	Exchange of Gramicidin between Lipid Bilayers: Implications for the Mechanism of Channel Formation. Biophysical Journal, 2017, 113, 1757-1767.	0.2	18
44	Computational Lipidomics of the Neuronal Plasma Membrane. Biophysical Journal, 2017, 113, 2271-2280.	0.2	197
45	Ganglioside-Lipid and Ganglioside-Protein Interactions Revealed by Coarse-Grained and Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2017, 121, 3262-3275.	1.2	81
46	Ganglioside and Protein-Ganglioside Interactions in Martini and Atomistic Molecular Dynamics Simulations. Biophysical Journal, 2016, 110, 254a.	0.2	0
47	Curvature-Induced Lipid Sorting in Plasma Membrane Tethers. Biophysical Journal, 2016, 110, 580a.	0.2	0
48	In Silico Modeling of Biologically Complex Membranes. Biophysical Journal, 2016, 110, 83a.	0.2	0
49	Computational â€˜microscopyâ€™ of cellular membranes. Journal of Cell Science, 2016, 129, 257-68.	1.2	119
50	Martini straight: Boosting performance using a shorter cutoff and GPUs. Computer Physics Communications, 2016, 199, 1-7.	3.0	352
51	Computational Lipidomics and the Lipid Organization of Cell Envelopes. Biophysical Journal, 2015, 108, 342a.	0.2	0
52	Parameters for Martini sterols and hopanoids based on a virtual-site description. Journal of Chemical Physics, 2015, 143, 243152.	1.2	125
53	Lipid Organization of the Plasma Membrane. Biophysical Journal, 2015, 108, 358a.	0.2	7
54	Martini Coarse-Grained Force Field: Extension to DNA. Journal of Chemical Theory and Computation, 2015, 11, 3932-3945.	2.3	239

#	Article	IF	Citations
55	Computational Lipidomics with insane: A Versatile Tool for Generating Custom Membranes for Molecular Simulations. Journal of Chemical Theory and Computation, 2015, 11, 2144-2155.	2.3	847
56	CHARMM-GUI Martini Maker for Coarse-Grained Simulations with the Martini Force Field. Journal of Chemical Theory and Computation, 2015, 11, 4486-4494.	2.3	340
57	Dry Martini, a Coarse-Grained Force Field for Lipid Membrane Simulations with Implicit Solvent. Journal of Chemical Theory and Computation, 2015, 11, 260-275.	2.3	236
58	The power of coarse graining in biomolecular simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 225-248.	6.2	423
59	Volatile anesthetics inhibit sodium channels without altering bulk lipid bilayer properties. Journal of General Physiology, 2014, 144, 545-560.	0.9	25
60	Global structural changes of an ion channel during its gating are followed by ion mobility mass spectrometry. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 17170-17175.	3.3	63
61	Lipid Organization of the Plasma Membrane. Journal of the American Chemical Society, 2014, 136, 14554-14559.	6.6	734
62	Phytochemicals Perturb Membranes and Promiscuously Alter Protein Function. ACS Chemical Biology, 2014, 9, 1788-1798.	1.6	241
63	The activation mode of the mechanosensitive ion channel, MscL, by lysophosphatidylcholine differs from tensionâ€induced gating. FASEB Journal, 2014, 28, 4292-4302.	0.2	42
64	Coarse-Grained Modeling of DNA-Vesicle Systems with the Martini Force Field. Biophysical Journal, 2014, 106, 803a.	0.2	1
65	Membrane Dependence of the Mechanosensitive Channel of Large Conductance. Biophysical Journal, 2014, 106, 38a.	0.2	1
66	Phytochemicals Promiscuously Alter Membrane Protein Function and Bilayer Properties. Biophysical Journal, 2013, 104, 93a.	0.2	0
67	Covering All the Bases: A Martini Coarse-Grained Force Field for DNA. Biophysical Journal, 2013, 104, 169a.	0.2	1
68	Coarse-Grained Molecular Dynamics Simulations Reveal the Membrane Dependence of MscL Gating. Biophysical Journal, 2013, 104, 663a.	0.2	0
69	Mixing MARTINI: Electrostatic Coupling in Hybrid Atomisticâ€“Coarse-Grained Biomolecular Simulations. Journal of Physical Chemistry B, 2013, 117, 3516-3530.	1.2	145
70	Whole Cell Screen for Inhibitors of pH Homeostasis in Mycobacterium tuberculosis. PLoS ONE, 2013, 8, e68942.	1.1	60
71	Gramicidin A Backbone and Side Chain Dynamics Evaluated by Molecular Dynamics Simulations and Nuclear Magnetic Resonance Experiments. II: Nuclear Magnetic Resonance Experiments. Journal of Physical Chemistry B, 2011, 115, 7427-7432.	1.2	5
72	Gramicidin A Backbone and Side Chain Dynamics Evaluated by Molecular Dynamics Simulations and Nuclear Magnetic Resonance Experiments. I: Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 7417-7426.	1.2	31

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73	Alcohol's Effects on Lipid Bilayer Properties. Biophysical Journal, 2011, 101, 847-855.	0.2	133
74	Exchange of Gramicidin between Lipid Bilayers: Implications for the Mechanism of Channel Formation and Gating. Biophysical Journal, 2011, 100, 501a.	0.2	1
75	Effects of Fluorinated Alcohols on Lipid Bilayers Properties. Biophysical Journal, 2011, 100, 500a.	0.2	0
76	Antidepressants Modify Lipid Bilayer Properties. Biophysical Journal, 2011, 100, 500a.	0.2	0
77	Effects of green tea catechins on gramicidin channel function and inferred changes in bilayer properties. FEBS Letters, 2011, 585, 3101-3105.	1.3	22
78	Gramicidin-based Fluorescence Assay; for Determining Small Molecules Potential for Modifying Lipid Bilayer Properties. Journal of Visualized Experiments, 2010, , .	0.2	30
79	Lipid bilayer regulation of membrane protein function: gramicidin channels as molecular force probes. Journal of the Royal Society Interface, 2010, 7, 373-395.	1.5	265
80	Screening for Small Molecules' Bilayer-Modifying Potential Using a Gramicidin-Based Fluorescence Assay. Assay and Drug Development Technologies, 2010, 8, 427-436.	0.6	60
81	Antidepressants Modify Lipid Bilayer Properties. Biophysical Journal, 2010, 98, 479a-480a.	0.2	0
82	High Throughput Gramicidin-Based Fluorescence Assay to Screen for Small Molecules' Bilayer-Perturbing Potential. Biophysical Journal, 2010, 98, 479a.	0.2	0
83	Evaluating Gramicidin A Channel Backbone Dynamics by Molecular Dynamics and Nuclear Magnetic Resonance. Biophysical Journal, 2009, 96, 152a-153a.	0.2	0
84	Protein Domain Prediction. Methods in Molecular Biology, 2008, 426, 117-143.	0.4	11
85	Preparation of Artificial Bilayers for Electrophysiology Experiments. Journal of Visualized Experiments, 2008, , .	0.2	7
86	Single Molecule Methods for Monitoring Changes in Bilayer Elastic Properties. Journal of Visualized Experiments, 2008, , .	0.2	3
87	The Inhibitory Effect of (â˜)-Epigallocatechin Gallate on Activation of the Epidermal Growth Factor Receptor Is Associated with Altered Lipid Order in HT29 Colon Cancer Cells. Cancer Research, 2007, 67, 6493-6501.	0.4	189
88	Curcumin is a Modulator of Bilayer Material Properties. Biochemistry, 2007, 46, 10384-10391.	1.2	132