Himanshu Khandelia

List of Publications by Year
in descending order

77 papers	2,187 citations	257429 24 h-index	265191 42 g-index
83 all docs	83 docs citations	83 times ranked	3017 citing authors

#	Article	IF	Citations
1	Triglyceride Blisters in Lipid Bilayers: Implications for Lipid Droplet Biogenesis and the Mobile Lipid Signal in Cancer Cell Membranes. PLoS ONE, 2010, 5, e12811.	2.5	138
2	Neurological disease mutations compromise a C-terminal ion pathway in the Na+/K+-ATPase. Nature, 2010, 467, 99-102.	27.8	125
3	The impact of peptides on lipid membranes. Biochimica Et Biophysica Acta - Biomembranes, 2008, 1778, 1528-1536.	2.6	124
4	Lipid Gymnastics: Evidence of Complete Acyl Chain Reversal in Oxidized Phospholipids from Molecular Simulations. Biophysical Journal, 2009, 96, 2734-2743.	0.5	117
5	Molecular dynamics simulations of the interactions of medicinal plant extracts and drugs with lipid bilayer membranes. FEBS Journal, 2013, 280, 2785-2805.	4.7	98
6	Molecular mechanism of the allosteric enhancement of the umami taste sensation. FEBS Journal, 2012, 279, 3112-3120.	4.7	88
7	Cationâ^Ï€ Interactions Stabilize the Structure of the Antimicrobial Peptide Indolicidin near Membranes:Â Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 242-250.	2.6	83
8	Structure of the antimicrobial Î²-hairpin peptide protegrin-1 in a DLPC lipid bilayer investigated by molecular dynamics simulation. Biochimica Et Biophysica Acta - Biomembranes, 2007, 1768, 509-520.	2.6	56
9	The N Terminus of Sarcolipin Plays an Important Role in Uncoupling Sarco-endoplasmic Reticulum Ca2+-ATPase (SERCA) ATP Hydrolysis from Ca2+ Transport. Journal of Biological Chemistry, 2015, 290, 14057-14067.	3.4	56
10	Membrane Tubulation in Lipid Vesicles Triggered by the Local Application of Calcium Ions. Langmuir, 2017, 33, 11010-11017.	3.5	51
11	Molecular dynamics simulations of helical antimicrobial peptides in SDS micelles: What do point mutations achieve?. Peptides, 2005, 26, 2037-2049.	2.4	50
12	Inclusion of Terpenoid Plant Extracts in Lipid Bilayers Investigated by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 15825-15831.	2.6	44
13	Correlation between simulated physicochemical properties and hemolycity of protegrin-like antimicrobial peptides: Predicting experimental toxicity. Peptides, 2008, 29, 1085-1093.	2.4	42
14	Driving engineering of novel antimicrobial peptides from simulations of peptideâ€“micelle interactions. Biochimica Et Biophysica Acta - Biomembranes, 2006, 1758, 1224-1234.	2.6	41
15	How can a Î²-sheet peptide be both a potent antimicrobial and harmfully toxic? Molecular dynamics simulations of protegrin-1 in micelles. Biopolymers, 2006, 84, 219-231.	2.4	41
16	High-Affinity Small Moleculeâ^Phospholipid Complex Formation: Binding of Siramesine to Phosphatidic Acid. Journal of the American Chemical Society, 2008, 130, 12953-12960.	13.7	38
17	Tuning of the Na,K-ATPase by the beta subunit. Scientific Reports, 2016, 6, 20442.	3.3	37
18	Molecular dynamics investigation of the influence of anionic and zwitterionic interfaces on antimicrobial peptidesâ€™ structure: Implications for peptide toxicity and activity. Peptides, 2006, 27, 1192-1200.	2.4	35

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19	Pairing of cholesterol with oxidized phospholipid species in lipid bilayers. Soft Matter, 2014, 10, 639-647.	2.7	35
20	Accelerating All-Atom MD Simulations of Lipids Using a Modified Virtual-Sites Technique. Journal of Chemical Theory and Computation, 2014, 10, 5690-5695.	5.3	34
21	Faster Simulations with a 5 fs Time Step for Lipids in the CHARMM Force Field. Journal of Chemical Theory and Computation, 2018, 14, 3342-3350.	5.3	34
22	Interaction of Salicylate and a Terpenoid Plant Extract with Model Membranes: Reconciling Experiments and Simulations. Biophysical Journal, 2010, 99, 3887-3894.	0.5	30
23	Molecular Dynamics Simulations of the Helical Antimicrobial Peptide Ovispirin-1 in a Zwitterionic Dodecylphosphocholine Micelle:â€‰ Insights into Host-Cell Toxicity. Journal of Physical Chemistry B, 2005, 109, 12990-12996.	2.6	28
24	Interdisciplinary Synergy to Reveal Mechanisms of Annexin-Mediated Plasma Membrane Shaping and Repair. Cells, 2020, 9, 1029.	4.1	28
25	Annexin A4 trimers are recruited by high membrane curvatures in giant plasma membrane vesicles. Soft Matter, 2021, 17, 308-318.	2.7	28
26	Selective chemical binding enhances cesium tolerance in plants through inhibition of cesium uptake. Scientific Reports, 2015, 5, 8842.	3.3	27
27	Clearance of activityâ€evoked K⁺ transients and associated glia cell swelling occur independently of <scp>AQP4</scp>: A study with an isoformâ€selective <scp>AQP4</scp> inhibitor. Glia, 2021, 69, 28-41.	4.9	27
28	Interaction of N-terminal peptide analogues of the Na+,K+-ATPase with membranes. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1282-1291.	2.6	26
29	Distribution of Neutral Lipids in the Lipid Droplet Core. Journal of Physical Chemistry B, 2014, 118, 11145-11151.	2.6	24
30	Quantifying the Relationship between Curvature and Electric Potential in Lipid Bilayers. Journal of Physical Chemistry B, 2016, 120, 4812-4817.	2.6	24
31	The CAPOS mutation in ATP1A3 alters Na/K-ATPase function and results in auditory neuropathy which has implications for management. Human Genetics, 2018, 137, 111-127.	3.8	24
32	Relative free energy of binding between antimicrobial peptides and SDS or DPC micelles. Molecular Simulation, 2009, 35, 986-997.	2.0	23
33	To Gate or Not To Gate: Using Molecular Dynamics Simulations To Morph Gated Plant Aquaporins into Constitutively Open Conformations. Journal of Physical Chemistry B, 2009, 113, 5239-5244.	2.6	23
34	Protein Kinase A (PKA) Phosphorylation of Na+/K+-ATPase Opens Intracellular C-terminal Water Pathway Leading to Third Na+-binding site in Molecular Dynamics Simulations*. Journal of Biological Chemistry, 2012, 287, 15959-15965.	3.4	23
35	Molecular Mechanism of Na⁺,K⁺-ATPase Malfunction in Mutations Characteristic of Adrenal Hypertension. Biochemistry, 2014, 53, 746-754.	2.5	23
36	Lipid Structure in Triolein Lipid Droplets. Journal of Physical Chemistry B, 2014, 118, 10335-10340.	2.6	22

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37	The effects of globotriaosylceramide tail saturation level on bilayer phases. Soft Matter, 2015, 11, 1352-1361.	2.7	22
38	Electrostatic Stabilization Plays a Central Role in Autoinhibitory Regulation of the Na+,K+-ATPase. Biophysical Journal, 2017, 112, 288-299.	0.5	22
39	A single K+-binding site in the crystal structure of the gastric proton pump. ELife, 2019, 8, .	6.0	22
40	Lipid peroxidation and water penetration in lipid bilayers: A W-band EPR study. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 510-517.	2.6	21
41	Perillyl alcohol: Dynamic interactions with the lipid bilayer and implications for long-term inhalational chemotherapy for gliomas. , 2016, 7, 1.		19
42	Propofol modulates the lipid phase transition and localizes near the headgroup of membranes. Chemistry and Physics of Lipids, 2013, 175-176, 84-91.	3.2	18
43	The role of caveolin-1 in lipid droplets and their biogenesis. Chemistry and Physics of Lipids, 2018, 211, 93-99.	3.2	18
44	EnCurv: Simple Technique of Maintaining Global Membrane Curvature in Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2021, 17, 1181-1193.	5.3	18
45	Design of new fluorescent cholesterol and ergosterol analogs: Insights from theory. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 2188-2199.	2.6	17
46	Reinforcing the membrane-mediated mechanism of action of the anti-tuberculosis candidate drug thioridazine with molecular simulations. Journal of Computer-Aided Molecular Design, 2014, 28, 123-134.	2.9	16
47	Phenothiazines alter plasma membrane properties andÂsensitize cancer cells to injury by inhibiting annexin-mediated repair. Journal of Biological Chemistry, 2021, 297, 101012.	3.4	16
48	Serine phosphorylation regulates the P-type potassium pump KdpFABC. ELife, 2020, 9, .	6.0	16
49	A novel role for methyl cysteinate, a cysteine derivative, in cesium accumulation in Arabidopsis thaliana. Scientific Reports, 2017, 7, 43170.	3.3	15
50	Lipid Configurations from Molecular Dynamics Simulations. Biophysical Journal, 2018, 114, 1895-1907.	0.5	14
51	Novel Ultrathin Membranes Composed of Organic Ions. Journal of Physical Chemistry Letters, 2013, 4, 1216-1220.	4.6	13
52	K+ binding and proton redistribution in the E2P state of the H+, K+-ATPase. Scientific Reports, 2018, 8, 12732.	3.3	13
53	Shuffled lipidation pattern and degree of lipidation determines the membrane interaction behavior of a linear cationic membrane-active peptide. Journal of Colloid and Interface Science, 2020, 578, 584-597.	9.4	13
54	Membrane accessibility of glutathione. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 2430-2436.	2.6	12

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55	Cholesterol binding to the sterol-sensing region of Niemann Pick C1 protein confines dynamics of its N-terminal domain. PLoS Computational Biology, 2020, 16, e1007554.	3.2	12
56	Conformations of double-headed, triple-tailed phospholipid oxidation lipid products in model membranes. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 1700-1706.	2.6	11
57	Structural design of intrinsically fluorescent oxysterols. Chemistry and Physics of Lipids, 2018, 212, 26-34.	3.2	11
58	On identifying collective displacements in apo-proteins that reveal eventual binding pathways. PLoS Computational Biology, 2019, 15, e1006665.	3.2	11
59	Different footprints of the Zika and dengue surface proteins on viral membranes. Soft Matter, 2018, 14, 5615-5621.	2.7	10
60	Insights into the role of cyclic ladderane lipids in bacteria from computer simulations. Chemistry and Physics of Lipids, 2014, 181, 76-82.	3.2	9
61	K+ Congeners That Do Not Compromise Na+ Activation of the Na+,K+-ATPase. Journal of Biological Chemistry, 2015, 290, 3720-3731.	3.4	9
62	The name of deliciousness and the gastrophysics behind it. Flavour, 2013, 2, .	2.3	8
63	Glutamate Water Gates in the Ion Binding Pocket of Na+ Bound Na+, K+-ATPase. Scientific Reports, 2017, 7, 39829.	3.3	8
64	Evidence for ATP Interaction with Phosphatidylcholine Bilayers. Langmuir, 2019, 35, 9944-9953.	3.5	8
65	Structural Basis for Binding of Potassium-Competitive Acid Blockers to the Gastric Proton Pump. Journal of Medicinal Chemistry, 2022, 65, 7843-7853.	6.4	8
66	Tension moderation and fluctuation spectrum in simulated lipid membranes under an applied electric potential. Journal of Chemical Physics, 2013, 139, 164902.	3.0	7
67	Interaction of the mononucleotide UMP with a fluid phospholipid bilayer. Soft Matter, 2019, 15, 8129-8136.	2.7	6
68	Long chain sphingomyelin depletes cholesterol from the cytoplasmic leaflet in asymmetric lipid membranes. RSC Advances, 2021, 11, 22677-22682.	3.6	5
69	Magic mushroom extracts in lipid membranes. Biochimica Et Biophysica Acta - Biomembranes, 2022, 1864, 183957.	2.6	5
70	An Intracellular Pathway Controlled by the N-terminus of the Pump Subunit Inhibits the Bacterial KdpFABC Ion Pump in High K+ Conditions. Journal of Molecular Biology, 2021, 433, 167008.	4.2	3
71	Thermodynamic Investigation of the Mechanism of Heat Production During Membrane Depolarization. Journal of Physical Chemistry B, 2020, 124, 2815-2822.	2.6	1
72	The Elusive Proton in the Gastric Proton Potassium ATPase. Biophysical Journal, 2018, 114, 146a.	0.5	0

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73	Mechanism of Cholesterol Sensing in the Niemann Pick Protein (NPC1) using Molecular Dynamics Simulations. Biophysical Journal, 2019, 116, 300a.	0.5	0
74	Title is missing!. , 2020, 16, e1007554.		0
75	Title is missing!. , 2020, 16, e1007554.		0
76	Title is missing!. , 2020, 16, e1007554.		0
77	Title is missing!. , 2020, 16, e1007554.		0