

Himanshu Khandelia

List of Publications by Citations

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71
papers

1,678
citations

23
h-index

38
g-index

83
ext. papers

1,968
ext. citations

4.9
avg, IF

5.02
L-index

#	Paper	IF	Citations
71	The impact of peptides on lipid membranes. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2008 , 1778, 1528-36	3.8	111
70	Lipid gymnastics: evidence of complete acyl chain reversal in oxidized phospholipids from molecular simulations. <i>Biophysical Journal</i> , 2009 , 96, 2734-43	2.9	109
69	Neurological disease mutations compromise a C-terminal ion pathway in the Na(+)/K(+)-ATPase. <i>Nature</i> , 2010 , 467, 99-102	50.4	105
68	Triglyceride blisters in lipid bilayers: implications for lipid droplet biogenesis and the mobile lipid signal in cancer cell membranes. <i>PLoS ONE</i> , 2010 , 5, e12811	3.7	100
67	Molecular dynamics simulations of the interactions of medicinal plant extracts and drugs with lipid bilayer membranes. <i>FEBS Journal</i> , 2013 , 280, 2785-805	5.7	80
66	Cation- π interactions stabilize the structure of the antimicrobial peptide indolicidin near membranes: molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 242-50	3.4	71
65	Molecular mechanism of the allosteric enhancement of the umami taste sensation. <i>FEBS Journal</i> , 2012 , 279, 3112-20	5.7	66
64	Structure of the antimicrobial beta-hairpin peptide protegrin-1 in a DLPC lipid bilayer investigated by molecular dynamics simulation. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2007 , 1768, 509-20	3.8	50
63	The N Terminus of Sarcolipin Plays an Important Role in Uncoupling Sarco-endoplasmic Reticulum Ca ²⁺ -ATPase (SERCA) ATP Hydrolysis from Ca ²⁺ Transport. <i>Journal of Biological Chemistry</i> , 2015 , 290, 14057-67	5.4	41
62	Membrane Tubulation in Lipid Vesicles Triggered by the Local Application of Calcium Ions. <i>Langmuir</i> , 2017 , 33, 11010-11017	4	39
61	How can a beta-sheet peptide be both a potent antimicrobial and harmfully toxic? Molecular dynamics simulations of protegrin-1 in micelles. <i>Biopolymers</i> , 2006 , 84, 219-31	2.2	39
60	Driving engineering of novel antimicrobial peptides from simulations of peptide-micelle interactions. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2006 , 1758, 1224-34	3.8	37
59	Inclusion of terpenoid plant extracts in lipid bilayers investigated by molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 15825-31	3.4	36
58	Molecular dynamics simulations of helical antimicrobial peptides in SDS micelles: what do point mutations achieve?. <i>Peptides</i> , 2005 , 26, 2037-49	3.8	36
57	Correlation between simulated physicochemical properties and hemolysis of protegrin-like antimicrobial peptides: predicting experimental toxicity. <i>Peptides</i> , 2008 , 29, 1085-93	3.8	34
56	High-affinity small molecule-phospholipid complex formation: binding of siramesine to phosphatidic acid. <i>Journal of the American Chemical Society</i> , 2008 , 130, 12953-60	16.4	34
55	Molecular dynamics investigation of the influence of anionic and zwitterionic interfaces on antimicrobial peptides structure: implications for peptide toxicity and activity. <i>Peptides</i> , 2006 , 27, 1192-200	3.8	32

54	Pairing of cholesterol with oxidized phospholipid species in lipid bilayers. <i>Soft Matter</i> , 2014 , 10, 639-47	3.6	29
53	Tuning of the Na,K-ATPase by the beta subunit. <i>Scientific Reports</i> , 2016 , 6, 20442	4.9	29
52	Interaction of salicylate and a terpenoid plant extract with model membranes: reconciling experiments and simulations. <i>Biophysical Journal</i> , 2010 , 99, 3887-94	2.9	28
51	Accelerating All-Atom MD Simulations of Lipids Using a Modified Virtual-Sites Technique. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5690-5	6.4	26
50	Molecular dynamics simulations of the helical antimicrobial peptide ovispirin-1 in a zwitterionic dodecylphosphocholine micelle: insights into host-cell toxicity. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 12990-6	3.4	26
49	Faster Simulations with a 5 fs Time Step for Lipids in the CHARMM Force Field. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 3342-3350	6.4	24
48	Interaction of N-terminal peptide analogues of the Na,K-ATPase with membranes. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018 , 1860, 1282-1291	3.8	22
47	To gate or not to gate: using molecular dynamics simulations to morph gated plant aquaporins into constitutively open conformations. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 5239-44	3.4	22
46	Molecular mechanism of Na(+),K(+)-ATPase malfunction in mutations characteristic of adrenal hypertension. <i>Biochemistry</i> , 2014 , 53, 746-54	3.2	21
45	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. <i>Journal of Biological Chemistry</i> , 2012 , 287, 15959-65	5.4	21
44	Quantifying the Relationship between Curvature and Electric Potential in Lipid Bilayers. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 4812-7	3.4	21
43	Selective chemical binding enhances cesium tolerance in plants through inhibition of cesium uptake. <i>Scientific Reports</i> , 2015 , 5, 8842	4.9	19
42	The effects of globotriaosylceramide tail saturation level on bilayer phases. <i>Soft Matter</i> , 2015 , 11, 1352-61	3.6	18
41	The CAPOS mutation in ATP1A3 alters Na/K-ATPase function and results in auditory neuropathy which has implications for management. <i>Human Genetics</i> , 2018 , 137, 111-127	6.3	17
40	Lipid structure in triolein lipid droplets. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 10335-40	3.4	17
39	Electrostatic Stabilization Plays a Central Role in Autoinhibitory Regulation of the Na,K-ATPase. <i>Biophysical Journal</i> , 2017 , 112, 288-299	2.9	16
38	Distribution of neutral lipids in the lipid droplet core. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 11145-53	3.4	16
37	Propofol modulates the lipid phase transition and localizes near the headgroup of membranes. <i>Chemistry and Physics of Lipids</i> , 2013 , 175-176, 84-91	3.7	16

36	Design of new fluorescent cholesterol and ergosterol analogs: Insights from theory. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2015 , 1848, 2188-99	3.8	16
35	Perillyl alcohol: Dynamic interactions with the lipid bilayer and implications for long-term inhalational chemotherapy for gliomas. <i>Surgical Neurology International</i> , 2016 , 7, 1	1	16
34	Reinforcing the membrane-mediated mechanism of action of the anti-tuberculosis candidate drug thioridazine with molecular simulations. <i>Journal of Computer-Aided Molecular Design</i> , 2014 , 28, 123-34	4.2	15
33	Lipid peroxidation and water penetration in lipid bilayers: a W-band EPR study. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2013 , 1828, 510-7	3.8	14
32	Interdisciplinary Synergy to Reveal Mechanisms of Annexin-Mediated Plasma Membrane Shaping and Repair. <i>Cells</i> , 2020 , 9,	7.9	13
31	Clearance of activity-evoked K transients and associated glia cell swelling occur independently of AQP4: A study with an isoform-selective AQP4 inhibitor. <i>Glia</i> , 2021 , 69, 28-41	9	13
30	A novel role for methyl cysteinate, a cysteine derivative, in cesium accumulation in <i>Arabidopsis thaliana</i> . <i>Scientific Reports</i> , 2017 , 7, 43170	4.9	11
29	A single K-binding site in the crystal structure of the gastric proton pump. <i>ELife</i> , 2019 , 8,	8.9	11
28	The role of caveolin-1 in lipid droplets and their biogenesis. <i>Chemistry and Physics of Lipids</i> , 2018 , 211, 93-99	3.7	11
27	Novel Ultrathin Membranes Composed of Organic Ions. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 1216-20	6.4	10
26	Conformations of double-headed, triple-tailed phospholipid oxidation lipid products in model membranes. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2013 , 1828, 1700-6	3.8	10
25	Annexin A4 trimers are recruited by high membrane curvatures in giant plasma membrane vesicles. <i>Soft Matter</i> , 2021 , 17, 308-318	3.6	10
24	Lipid Configurations from Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2018 , 114, 1895-1907	2.9	9
23	Insights into the role of cyclic ladderane lipids in bacteria from computer simulations. <i>Chemistry and Physics of Lipids</i> , 2014 , 181, 76-82	3.7	9
22	Membrane accessibility of glutathione. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2015 , 1848, 2430-6.8	6.8	8
21	Structural design of intrinsically fluorescent oxysterols. <i>Chemistry and Physics of Lipids</i> , 2018 , 212, 26-34	3.7	8
20	K ⁺ congeners that do not compromise Na ⁺ activation of the Na ⁺ ,K ⁺ -ATPase: hydration of the ion binding cavity likely controls ion selectivity. <i>Journal of Biological Chemistry</i> , 2015 , 290, 3720-31	5.4	8
19	Relative free energy of binding between antimicrobial peptides and SDS or DPC micelles. <i>Molecular Simulation</i> , 2009 , 35, 986-997	2	8

18	Serine phosphorylation regulates the P-type potassium pump KdpFABC. <i>ELife</i> , 2020 , 9,	8.9	8
17	Tension moderation and fluctuation spectrum in simulated lipid membranes under an applied electric potential. <i>Journal of Chemical Physics</i> , 2013 , 139, 164902	3.9	7
16	Glutamate Water Gates in the Ion Binding Pocket of Na Bound Na, K-ATPase. <i>Scientific Reports</i> , 2017 , 7, 39829	4.9	7
15	On identifying collective displacements in apo-proteins that reveal eventual binding pathways. <i>PLoS Computational Biology</i> , 2019 , 15, e1006665	5	7
14	Shuffled lipidation pattern and degree of lipidation determines the membrane interaction behavior of a linear cationic membrane-active peptide. <i>Journal of Colloid and Interface Science</i> , 2020 , 578, 584-597	9.3	6
13	Evidence for ATP Interaction with Phosphatidylcholine Bilayers. <i>Langmuir</i> , 2019 , 35, 9944-9953	4	6
12	The name of deliciousness and the gastrophysics behind it. <i>Flavour</i> , 2013 , 2,		6
11	EnCurv: Simple Technique of Maintaining Global Membrane Curvature in Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 1181-1193	6.4	6
10	K binding and proton redistribution in the EP state of the H, K-ATPase. <i>Scientific Reports</i> , 2018 , 8, 12732	4.9	5
9	Different footprints of the Zika and dengue surface proteins on viral membranes. <i>Soft Matter</i> , 2018 , 14, 5615-5621	3.6	4
8	Cholesterol binding to the sterol-sensing region of Niemann Pick C1 protein confines dynamics of its N-terminal domain. <i>PLoS Computational Biology</i> , 2020 , 16, e1007554	5	2
7	Thermodynamic Investigation of the Mechanism of Heat Production During Membrane Depolarization. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 2815-2822	3.4	1
6	Interaction of the mononucleotide UMP with a fluid phospholipid bilayer. <i>Soft Matter</i> , 2019 , 15, 8129-8136	3.6	1
5	Long chain sphingomyelin depletes cholesterol from the cytoplasmic leaflet in asymmetric lipid membranes.. <i>RSC Advances</i> , 2021 , 11, 22677-22682	3.7	1
4	An Intracellular Pathway Controlled by the N-terminus of the Pump Subunit Inhibits the Bacterial KdpFABC Ion Pump in High K Conditions. <i>Journal of Molecular Biology</i> , 2021 , 433, 167008	6.5	1
3	Phenothiazines alter plasma membrane properties and sensitize cancer cells to injury by inhibiting annexin-mediated repair. <i>Journal of Biological Chemistry</i> , 2021 , 297, 101012	5.4	0
2	Magic mushroom extracts in lipid membranes.. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2022 , 1839-58	5.8	0
1	Multi-scale Modeling of Biomimetic Membranes 2011 , 157-185		

