Himanshu Khandelia

List of Publications by Year in Descending Order

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	Magic mushroom extracts in lipid membranes.. *Biochimica Et Biophysica Acta - Biomembranes*, **2022**, 183958	3.8	0
70	Clearance of activity-evoked K transients and associated glia cell swelling occur independently of AQP4: A study with an isoform-selective AQP4 inhibitor. *Glia*, **2021**, 69, 28-41	9	13
69	Annexin A4 trimers are recruited by high membrane curvatures in giant plasma membrane vesicles. *Soft Matter*, **2021**, 17, 308-318	3.6	10
68	Long chain sphingomyelin depletes cholesterol from the cytoplasmic leaflet in asymmetric lipid membranes.. *RSC Advances*, **2021**, 11, 22677-22682	3.7	1
67	EnCurv: Simple Technique of Maintaining Global Membrane Curvature in Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 1181-1193	6.4	6
66	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	6.5	1
65	Phenothiazines alter plasma membrane properties and sensitize cancer cells to injury by inhibiting annexin-mediated repair. *Journal of Biological Chemistry*, **2021**, 297, 101012	5.4	0
64	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	9.3	6
63	Thermodynamic Investigation of the Mechanism of Heat Production During Membrane Depolarization. *Journal of Physical Chemistry B*, **2020**, 124, 2815-2822	3.4	1
62	Interdisciplinary Synergy to Reveal Mechanisms of Annexin-Mediated Plasma Membrane Shaping and Repair. *Cells*, **2020**, 9,	7.9	13
61	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	5	2
60	Serine phosphorylation regulates the P-type potassium pump KdpFABC. *ELife*, **2020**, 9,	8.9	8
59	Evidence for ATP Interaction with Phosphatidylcholine Bilayers. *Langmuir*, **2019**, 35, 9944-9953	4	6
58	A single K-binding site in the crystal structure of the gastric proton pump. *ELife*, **2019**, 8,	8.9	11
57	Interaction of the mononucleotide UMP with a fluid phospholipid bilayer. *Soft Matter*, **2019**, 15, 8129-8136	3.6	1
56	On identifying collective displacements in apo-proteins that reveal eventual binding pathways. *PLoS Computational Biology*, **2019**, 15, e1006665	5	7
55	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	6.3	17

54	Structural design of intrinsically fluorescent oxysterols. *Chemistry and Physics of Lipids*, **2018**, 212, 26-34	3.7	8
53	Lipid Configurations from Molecular Dynamics Simulations. *Biophysical Journal*, **2018**, 114, 1895-1907	2.9	9
52	Interaction of N-terminal peptide analogues of the Na,K-ATPase with membranes. *Biochimica Et Biophysica Acta - Biomembranes*, **2018**, 1860, 1282-1291	3.8	22
51	Different footprints of the Zika and dengue surface proteins on viral membranes. *Soft Matter*, **2018**, 14, 5615-5621	3.6	4
50	The role of caveolin-1 in lipid droplets and their biogenesis. *Chemistry and Physics of Lipids*, **2018**, 211, 93-99	3.7	11
49	K binding and proton redistribution in the EP state of the H, K-ATPase. *Scientific Reports*, **2018**, 8, 12732	4.9	5
48	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	6.4	24
47	Electrostatic Stabilization Plays a Central Role in Autoinhibitory Regulation of the Na,K-ATPase. *Biophysical Journal*, **2017**, 112, 288-299	2.9	16
46	A novel role for methyl cysteinate, a cysteine derivative, in cesium accumulation in Arabidopsis thaliana. *Scientific Reports*, **2017**, 7, 43170	4.9	11
45	Membrane Tubulation in Lipid Vesicles Triggered by the Local Application of Calcium Ions. *Langmuir*, **2017**, 33, 11010-11017	4	39
44	Glutamate Water Gates in the Ion Binding Pocket of Na Bound Na, K-ATPase. *Scientific Reports*, **2017**, 7, 39829	4.9	7
43	Perillyl alcohol: Dynamic interactions with the lipid bilayer and implications for long-term inhalational chemotherapy for gliomas. *Surgical Neurology International*, **2016**, 7, 1	1	16
42	Tuning of the Na,K-ATPase by the beta subunit. *Scientific Reports*, **2016**, 6, 20442	4.9	29
41	Quantifying the Relationship between Curvature and Electric Potential in Lipid Bilayers. *Journal of Physical Chemistry B*, **2016**, 120, 4812-7	3.4	21
40	Selective chemical binding enhances cesium tolerance in plants through inhibition of cesium uptake. *Scientific Reports*, **2015**, 5, 8842	4.9	19
39	Membrane accessibility of glutathione. *Biochimica Et Biophysica Acta - Biomembranes*, **2015**, 1848, 2430-6	3.8	8
38	Design of new fluorescent cholesterol and ergosterol analogs: Insights from theory. *Biochimica Et Biophysica Acta - Biomembranes*, **2015**, 1848, 2188-99	3.8	16
37	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, 14057-67	5.4	41

36	K+ congeners that do not compromise Na+ activation of the Na+,K+-ATPase: hydration of the ion binding cavity likely controls ion selectivity. *Journal of Biological Chemistry*, **2015**, 290, 3720-31	5.4	8
35	The effects of globotriaosylceramide tail saturation level on bilayer phases. *Soft Matter*, **2015**, 11, 1352-61	3.6	18
34	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, 123-34	4.2	15
33	Pairing of cholesterol with oxidized phospholipid species in lipid bilayers. *Soft Matter*, **2014**, 10, 639-47	3.6	29
32	Molecular mechanism of Na(+),K(+)-ATPase malfunction in mutations characteristic of adrenal hypertension. *Biochemistry*, **2014**, 53, 746-54	3.2	21
31	Lipid structure in triolein lipid droplets. *Journal of Physical Chemistry B*, **2014**, 118, 10335-40	3.4	17
30	Accelerating All-Atom MD Simulations of Lipids Using a Modified Virtual-Sites Technique. *Journal of Chemical Theory and Computation*, **2014**, 10, 5690-5	6.4	26
29	Distribution of neutral lipids in the lipid droplet core. *Journal of Physical Chemistry B*, **2014**, 118, 11145-53	3.4	16
28	Insights into the role of cyclic ladderane lipids in bacteria from computer simulations. *Chemistry and Physics of Lipids*, **2014**, 181, 76-82	3.7	9
27	Novel Ultrathin Membranes Composed of Organic Ions. *Journal of Physical Chemistry Letters*, **2013**, 4, 1216-20	6.4	10
26	Propofol modulates the lipid phase transition and localizes near the headgroup of membranes. *Chemistry and Physics of Lipids*, **2013**, 175-176, 84-91	3.7	16
25	Conformations of double-headed, triple-tailed phospholipid oxidation lipid products in model membranes. *Biochimica Et Biophysica Acta - Biomembranes*, **2013**, 1828, 1700-6	3.8	10
24	Tension moderation and fluctuation spectrum in simulated lipid membranes under an applied electric potential. *Journal of Chemical Physics*, **2013**, 139, 164902	3.9	7
23	The name of deliciousness and the gastrophysics behind it. *Flavour*, **2013**, 2,		6
22	Molecular dynamics simulations of the interactions of medicinal plant extracts and drugs with lipid bilayer membranes. *FEBS Journal*, **2013**, 280, 2785-805	5.7	80
21	Lipid peroxidation and water penetration in lipid bilayers: a W-band EPR study. *Biochimica Et Biophysica Acta - Biomembranes*, **2013**, 1828, 510-7	3.8	14
20	Molecular mechanism of the allosteric enhancement of the umami taste sensation. *FEBS Journal*, **2012**, 279, 3112-20	5.7	66
19	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, 15959-65	5.4	21

18	Multi-scale Modeling of Biomimetic Membranes **2011**, 157-185		
17	Neurological disease mutations compromise a C-terminal ion pathway in the Na(+)/K(+)-ATPase. *Nature*, **2010**, 467, 99-102	50.4	105
16	Triglyceride blisters in lipid bilayers: implications for lipid droplet biogenesis and the mobile lipid signal in cancer cell membranes. *PLoS ONE*, **2010**, 5, e12811	3.7	100
15	Interaction of salicylate and a terpenoid plant extract with model membranes: reconciling experiments and simulations. *Biophysical Journal*, **2010**, 99, 3887-94	2.9	28
14	Inclusion of terpenoid plant extracts in lipid bilayers investigated by molecular dynamics simulations. *Journal of Physical Chemistry B*, **2010**, 114, 15825-31	3.4	36
13	Relative free energy of binding between antimicrobial peptides and SDS or DPC micelles. *Molecular Simulation*, **2009**, 35, 986-997	2	8
12	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, 5239-44	3.4	22
11	Lipid gymnastics: evidence of complete acyl chain reversal in oxidized phospholipids from molecular simulations. *Biophysical Journal*, **2009**, 96, 2734-43	2.9	109
10	Correlation between simulated physicochemical properties and hemolycity of protegrin-like antimicrobial peptides: predicting experimental toxicity. *Peptides*, **2008**, 29, 1085-93	3.8	34
9	The impact of peptides on lipid membranes. *Biochimica Et Biophysica Acta - Biomembranes*, **2008**, 1778, 1528-36	3.8	111
8	High-affinity small molecule-phospholipid complex formation: binding of siramesine to phosphatidic acid. *Journal of the American Chemical Society*, **2008**, 130, 12953-60	16.4	34
7	Cation-pi interactions stabilize the structure of the antimicrobial peptide indolicidin near membranes: molecular dynamics simulations. *Journal of Physical Chemistry B*, **2007**, 111, 242-50	3.4	71
6	Structure of the antimicrobial beta-hairpin peptide protegrin-1 in a DLPC lipid bilayer investigated by molecular dynamics simulation. *Biochimica Et Biophysica Acta - Biomembranes*, **2007**, 1768, 509-20	3.8	50
5	How can a beta-sheet peptide be both a potent antimicrobial and harmfully toxic? Molecular dynamics simulations of protegrin-1 in micelles. *Biopolymers*, **2006**, 84, 219-31	2.2	39
4	Driving engineering of novel antimicrobial peptides from simulations of peptide-micelle interactions. *Biochimica Et Biophysica Acta - Biomembranes*, **2006**, 1758, 1224-34	3.8	37
3	Molecular dynamics investigation of the influence of anionic and zwitterionic interfaces on antimicrobial peptidesSstructure: implications for peptide toxicity and activity. *Peptides*, **2006**, 27, 1192-200	3.8	32
2	Molecular dynamics simulations of the helical antimicrobial peptide ovispirin-1 in a zwitterionic dodecylphosphocholine micelle: insights into host-cell toxicity. *Journal of Physical Chemistry B*, **2005**, 109, 12990-6	3.4	26
1	Molecular dynamics simulations of helical antimicrobial peptides in SDS micelles: what do point mutations achieve?. *Peptides*, **2005**, 26, 2037-49	3.8	36