Hanif M Khan

List of Publications by Year
in descending order

19 papers	916 citations	759233 12 h-index	839539 18 g-index
26 all docs	26 docs citations	26 times ranked	840 citing authors

#	Article	IF	Citations
1	Specificity of Loxosceles Î± clade phospholipase D enzymes for choline-containing lipids: Role of a conserved aromatic cage. PLoS Computational Biology, 2022, 18, e1009871.	3.2	6
2	Standard Binding Free Energy and Membrane Desorption Mechanism for a Phospholipase C. Journal of Chemical Information and Modeling, 2022, 62, 6602-6613.	5.4	8
3	Refinement of a cryo-EM structure of hERG: Bridging structure and function. Biophysical Journal, 2021, 120, 738-748.	0.5	5
4	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	19.0	557
5	Phospholipids in Motion: High-Resolution ³¹P NMR Field Cycling Studies. Journal of Physical Chemistry B, 2021, 125, 8827-8838.	2.6	5
6	Cryo-EM structure of the sodium-driven chloride/bicarbonate exchanger NDCBE. Nature Communications, 2021, 12, 5690.	12.8	24
7	Allosteric Coupling Between Drug Binding and the Aromatic Cassette in the Pore Domain of the hERG1 Channel: Implications for a State-Dependent Blockade. Frontiers in Pharmacology, 2020, 11, 914.	3.5	6
8	Capturing Cholineâ€“Aromatics Cationâ˜Ï€ Interactions in the MARTINI Force Field. Journal of Chemical Theory and Computation, 2020, 16, 2550-2560.	5.3	35
9	Interfacial Aromatics Mediating Cationâ˜Ï€ Interactions with Choline-Containing Lipids Can Contribute as Much to Peripheral Protein Affinity for Membranes as Aromatics Inserted below the Phosphates. Journal of Physical Chemistry Letters, 2019, 10, 3972-3977.	4.6	24
10	Cation-Ï€ Interactions between Methylated Ammonium Groups and Tryptophan in the CHARMM36 Additive Force Field. Journal of Chemical Theory and Computation, 2019, 15, 7-12.	5.3	58
11	Search and Subvert: Minimalist Bacterial Phosphatidylinositol-Specific Phospholipase C Enzymes. Chemical Reviews, 2018, 118, 8435-8473.	47.7	25
12	Improving the Force Field Description of Tyrosineâ€“Choline Cationâ˜Ï€ Interactions: QM Investigation of Phenolâ€“N(Me)₄⁺ Interactions. Journal of Chemical Theory and Computation, 2016, 12, 5585-5595.	5.3	39
13	A Role for Weak Electrostatic Interactions in Peripheral Membrane Protein Binding. Biophysical Journal, 2016, 110, 1367-1378.	0.5	47
14	Membrane Docking of the Synaptotagmin 7 C2A Domain: Computation Reveals Interplay between Electrostatic and Hydrophobic Contributions. Biochemistry, 2015, 54, 5696-5711.	2.5	21
15	Quantifying Transient Interactions between Bacillus Phosphatidylinositol-Specific Phospholipase-C and Phosphatidylcholine-Rich Vesicles. Journal of the American Chemical Society, 2015, 137, 14-17.	13.7	24
16	Two homologous neutrophil serine proteases bind to POPC vesicles with different affinities: When aromatic amino acids matter. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 3191-3202.	2.6	16
17	On the wear mechanism of thin nickel film during AFM-based scratching process using molecular dynamics. Journal of Mechanical Science and Technology, 2011, 25, 2111-2120.	1.5	15
18	High Strain Rate Induced Phenomenon in Thin Nickel Films. , 2010, , .		0

#	Article	IF	Citations
19	Atomistic modeling of scratching process based on Atomic Force Microscope: Effects of temperature. , 2010, , .		0