

Jigneshkumar Dahyabhai Prajapati

List of Publications by Year in descending order

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Version: 2024-02-01

22
papers

611
citations

687363

13
h-index

713466

21
g-index

22
all docs

22
docs citations

22
times ranked

643
citing authors

#	ARTICLE	IF	CITATIONS
1	How to Enter a Bacterium: Bacterial Porins and the Permeation of Antibiotics. <i>Chemical Reviews</i> , 2021, 121, 5158-5192.	47.7	103
2	Outer-membrane translocation of bulky small molecules by passive diffusion. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E2991-9.	7.1	70
3	Atomistic Modeling of Two-Dimensional Electronic Spectra and Excited-State Dynamics for a Light Harvesting 2 Complex. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1302-1313.	2.6	59
4	Role of Electroosmosis in the Permeation of Neutral Molecules: CymA and Cyclodextrin as an Example. <i>Biophysical Journal</i> , 2016, 110, 600-611.	0.5	55
5	Characterization of Ciprofloxacin Permeation Pathways across the Porin OmpC Using Metadynamics and a String Method. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4553-4566.	5.3	41
6	A Multidisciplinary Approach toward Identification of Antibiotic Scaffolds for <i>Acinetobacter baumannii</i> . <i>Structure</i> , 2019, 27, 268-280.e6.	3.3	41
7	DFTB/MM Molecular Dynamics Simulations of the FMO Light-Harvesting Complex. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8660-8667.	4.6	34
8	Exploration of Free Energy Surfaces Across a Membrane Channel Using Metadynamics and Umbrella Sampling. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2751-2765.	5.3	26
9	Enrofloxacin Permeation Pathways across the Porin OmpC. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1417-1426.	2.6	24
10	Dynamic interaction of fluoroquinolones with magnesium ions monitored using bacterial outer membrane nanopores. <i>Chemical Science</i> , 2020, 11, 10344-10353.	7.4	23
11	Molecular Interactions of Cephalosporins with the Deep Binding Pocket of the RND Transporter AcrB. <i>Journal of Physical Chemistry B</i> , 2019, 123, 4625-4635.	2.6	18
12	Environmental effects on the dynamics in the light-harvesting complexes LH2 and LH3 based on molecular simulations. <i>Chemical Physics</i> , 2018, 515, 141-151.	1.9	16
13	Computational Modeling of Ion Transport in Bulk and through a Nanopore Using the Drude Polarizable Force Field. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3188-3203.	5.4	16
14	Large Peptide Permeation Through a Membrane Channel: Understanding Protamine Translocation Through CymA from <i>Klebsiella Oxytoca</i> . <i>Angewandte Chemie - International Edition</i> , 2021, 60, 8089-8094.	13.8	15
15	Improved Sampling and Free Energy Estimates for Antibiotic Permeation through Bacterial Porins. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4564-4577.	5.3	15
16	BROMOCEA Code: An Improved Grand Canonical Monte Carlo/Brownian Dynamics Algorithm Including Explicit Atoms. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2401-2417.	5.3	14
17	Brownian Dynamics Approach Including Explicit Atoms for Studying Ion Permeation and Substrate Translocation across Nanopores. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6701-6713.	5.3	11
18	Voltage-Dependent Transport of Neutral Solutes through Nanopores: A Molecular View. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10718-10731.	2.6	8

#	ARTICLE	IF	CITATIONS
19	Millisecond-Long Simulations of Antibiotics Transport through Outer Membrane Channels. Journal of Chemical Theory and Computation, 2021, 17, 549-559.	5.3	8
20	Changes in Salt Concentration Modify the Translocation of Neutral Molecules through a β -CymA Nanopore in a Non-monotonic Manner. ACS Nano, 2022, 16, 7701-7712.	14.6	6
21	Atomistic Simulation of Molecules Interacting with Biological Nanopores: From Current Understanding to Future Directions. Journal of Physical Chemistry B, 0, , .	2.6	6
22	Permeation eines 5.1â€kDaâ€Peptides durch einen Proteinkanal: Molekulare Basis der Translokation von Protamin durch CymA aus Klebsiella Oxytoca **. Angewandte Chemie, 2021, 133, 8170-8175.	2.0	2