Jigneshkumar Dahyabhai Prajapati

List of Publications by Year
in descending order

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	Changes in Salt Concentration Modify the Translocation of Neutral Molecules through a Î”CymA Nanopore in a Non-monotonic Manner. ACS Nano, 2022, 16, 7701-7712.	14.6	6
2	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
3	How to Enter a Bacterium: Bacterial Porins and the Permeation of Antibiotics. Chemical Reviews, 2021, 121, 5158-5192.	47.7	103
4	Largeâ€Peptide Permeation Through a Membrane Channel: Understanding Protamine Translocation Through CymA from Klebsiella Oxytoca**. Angewandte Chemie - International Edition, 2021, 60, 8089-8094.	13.8	15
5	Improved Sampling and Free Energy Estimates for Antibiotic Permeation through Bacterial Porins. Journal of Chemical Theory and Computation, 2021, 17, 4564-4577.	5.3	15
6	Millisecond-Long Simulations of Antibiotics Transport through Outer Membrane Channels. Journal of Chemical Theory and Computation, 2021, 17, 549-559.	5.3	8
7	DFTB/MM Molecular Dynamics Simulations of the FMO Light-Harvesting Complex. Journal of Physical Chemistry Letters, 2020, 11, 8660-8667.	4.6	34
8	Voltage-Dependent Transport of Neutral Solutes through Nanopores: A Molecular View. Journal of Physical Chemistry B, 2020, 124, 10718-10731.	2.6	8
9	Dynamic interaction of fluoroquinolones with magnesium ions monitored using bacterial outer membrane nanopores. Chemical Science, 2020, 11, 10344-10353.	7.4	23
10	Computational Modeling of Ion Transport in Bulk and through a Nanopore Using the Drude Polarizable Force Field. Journal of Chemical Information and Modeling, 2020, 60, 3188-3203.	5.4	16
11	Exploration of Free Energy Surfaces Across a Membrane Channel Using Metadynamics and Umbrella Sampling. Journal of Chemical Theory and Computation, 2020, 16, 2751-2765.	5.3	26
12	Molecular Interactions of Cephalosporins with the Deep Binding Pocket of the RND Transporter AcrB. Journal of Physical Chemistry B, 2019, 123, 4625-4635.	2.6	18
13	A Multidisciplinary Approach toward Identification of Antibiotic Scaffolds for Acinetobacter baumannii. Structure, 2019, 27, 268-280.e6.	3.3	41
14	Enrofloxacin Permeation Pathways across the Porin OmpC. Journal of Physical Chemistry B, 2018, 122, 1417-1426.	2.6	24
15	Brownian Dynamics Approach Including Explicit Atoms for Studying Ion Permeation and Substrate Translocation across Nanopores. Journal of Chemical Theory and Computation, 2018, 14, 6701-6713.	5.3	11
16	Environmental effects on the dynamics in the light-harvesting complexes LH2 and LH3 based on molecular simulations. Chemical Physics, 2018, 515, 141-151.	1.9	16
17	Characterization of Ciprofloxacin Permeation Pathways across the Porin OmpC Using Metadynamics and a String Method. Journal of Chemical Theory and Computation, 2017, 13, 4553-4566.	5.3	41
18	BROMOCEA Code: An Improved Grand Canonical Monte Carlo/Brownian Dynamics Algorithm Including Explicit Atoms. Journal of Chemical Theory and Computation, 2016, 12, 2401-2417.	5.3	14

#	Article	IF	Citations
19	Role of Electroosmosis in the Permeation of Neutral Molecules: CymA and Cyclodextrin as an Example. Biophysical Journal, 2016, 110, 600-611.	0.5	55
20	Atomistic Modeling of Two-Dimensional Electronic Spectra and Excited-State Dynamics for a Light Harvesting 2 Complex. Journal of Physical Chemistry B, 2015, 119, 1302-1313.	2.6	59
21	Outer-membrane translocation of bulky small molecules by passive diffusion. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E2991-9.	7.1	70
22	Atomistic Simulation of Molecules Interacting with Biological Nanopores: From Current Understanding to Future Directions. Journal of Physical Chemistry B, 0, , .	2.6	6