Giacomo Fiorin

List of Publications by Year
in descending order

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38 papers	4,446 citations	304743 22 h-index	330143 37 g-index
41 all docs	41 docs citations	41 times ranked	5458 citing authors

#	Article	IF	Citations
1	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	3.0	1,548
2	Using collective variables to drive molecular dynamics simulations. Molecular Physics, 2013, 111, 3345-3362.	1.7	750
3	Exploring Multidimensional Free Energy Landscapes Using Time-Dependent Biases on Collective Variables. Journal of Chemical Theory and Computation, 2010, 6, 35-47.	5.3	366
4	Structure and mechanism of proton transport through the transmembrane tetrameric M2 protein bundle of the influenza A virus. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 15075-15080.	7.1	243
5	Structure and inhibition of the drug-resistant S31N mutant of the M2 ion channel of influenza A virus. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 1315-1320.	7.1	204
6	Structure of Water at Charged Interfaces: A Molecular Dynamics Study. Langmuir, 2014, 30, 8056-8065.	3.5	130
7	Molecular Dynamics Simulation Directed Rational Design of Inhibitors Targeting Drug-Resistant Mutants of Influenza A Virus M2. Journal of the American Chemical Society, 2011, 133, 12834-12841.	13.7	127
8	Functional Studies and Modeling of Pore-Lining Residue Mutants of the Influenza A Virus M2 Ion Channel. Biochemistry, 2010, 49, 696-708.	2.5	107
9	High-resolution structures of the M2 channel from influenza A virus reveal dynamic pathways for proton stabilization and transduction. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 14260-14265.	7.1	92
10	On the Role of Water in Peroxidase Catalysis: A Theoretical Investigation of HRP Compound I Formation. Journal of Physical Chemistry B, 2010, 114, 5161-5169.	2.6	89
11	Discovery of Novel Dual Inhibitors of the Wild-Type and the Most Prevalent Drug-Resistant Mutant, S31N, of the M2 Proton Channel from Influenza A Virus. Journal of Medicinal Chemistry, 2013, 56, 2804-2812.	6.4	88
12	Flipping in the Pore: Discovery of Dual Inhibitors That Bind in Different Orientations to the Wild-Type versus the Amantadine-Resistant S31N Mutant of the Influenza A Virus M2 Proton Channel. Journal of the American Chemical Society, 2014, 136, 17987-17995.	13.7	78
13	Transmembrane orientation and possible role of the fusogenic peptide from parainfluenza virus 5 (PIV5) in promoting fusion. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3958-3963.	7.1	65
14	Pore waters regulate ion permeation in a calcium release-activated calcium channel. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 17332-17337.	7.1	65
15	Supramolecular Polymerization of Benzene-1,3,5-tricarboxamide: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2014, 118, 5218-5228.	2.6	61
16	Molecular dynamics simulations of cholesterol-rich membranes using a coarse-grained force field for cyclic alkanes. Journal of Chemical Physics, 2015, 143, 243144.	3.0	55
17	Large-scale state-dependent membrane remodeling by a transporter protein. ELife, 2019, 8, .	6.0	42
18	Asp44 Stabilizes the Trp41 Gate of the M2 Proton Channel of Influenza A Virus. Structure, 2013, 21, 2033-2041.	3.3	34

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19	Hydrogen-Bonded Water Molecules in the M2 Channel of the Influenza A Virus Guide the Binding Preferences of Ammonium-Based Inhibitors. Journal of Physical Chemistry B, 2015, 119, 1173-1183.	2.6	33
20	Multiple Proton Confinement in the M2 Channel from the Influenza A Virus. Journal of Physical Chemistry C, 2010, 114, 20856-20863.	3.1	31
21	Binding of the Antitubercular Pro-Drug Isoniazid in the Heme Access Channel of Catalase-Peroxidase (KatG). A Combined Structural and Metadynamics Investigation. Journal of Physical Chemistry B, 2014, 118, 2924-2931.	2.6	27
22	Structural Refinement of Proteins by Restrained Molecular Dynamics Simulations with Non-interacting Molecular Fragments. PLoS Computational Biology, 2015, 11, e1004368.	3.2	26
23	Direct Derivation of Free Energies of Membrane Deformation and Other Solvent Density Variations From Enhanced Sampling Molecular Dynamics. Journal of Computational Chemistry, 2020, 41, 449-459.	3.3	26
24	SPICA Force Field for Proteins and Peptides. Journal of Chemical Theory and Computation, 2022, 18, 3204-3217.	5.3	21
25	Structural Characterization of Biomolecules through Atomistic Simulations Guided by DEER Measurements. Structure, 2019, 27, 359-370.e12.	3.3	20
26	Infrared and fluorescence assessment of the hydration status of the tryptophan gate in the influenza A M2 proton channel. Physical Chemistry Chemical Physics, 2016, 18, 28939-28950.	2.8	19
27	Exploring Histidine Conformations in the M2 Channel Lumen of the Influenza A Virus at Neutral pH via Molecular Simulations. Journal of Physical Chemistry Letters, 2013, 4, 3067-3071.	4.6	14
28	Coexistence of Lipid Phases Stabilizes Interstitial Water in the Outer Layer of Mammalian Skin. Biophysical Journal, 2020, 118, 1588-1601.	0.5	13
29	Data-guided Multi-Map variables for ensemble refinement of molecular movies. Journal of Chemical Physics, 2020, 153, 214102.	3.0	12
30	The Flu's Proton Escort. Science, 2010, 330, 456-458.	12.6	11
31	Dehydration of multilamellar fatty acid membranes: Towards a computational model of the stratum corneum. Journal of Chemical Physics, 2014, 141, 22D526.	3.0	9
32	Human Learning for Molecular Simulations: The Collective Variables Dashboard in VMD. Journal of Chemical Theory and Computation, 2022, 18, 1945-1956.	5.3	8
33	Different bonding type along each crystallographic axis: Computational study of poly(p -phenylene) Tj ETQq1 1 0.784314 rgBT /Overl	2.4	7
34	Mechanically Strong Polymer Sheets from Aligned Ultrahigh-Molecular-Weight Polyethylene Nanocomposites. Journal of Physical Chemistry Letters, 2018, 9, 2652-2658.	4.6	6
35	The challenge of stochastic StÃ¸rmerâ€“Verlet thermostats generating correct statistics. Journal of Chemical Physics, 2020, 153, 134101.	3.0	5
36	Aggregation of poly(<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 67 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML"><r	2.4	5

#	Article	IF	Citations
37	Shear response in crystalline models of poly(p-phenylene terephthalamide). Molecular Physics, 0, , e1948122.	1.7	3
38	Bringing discrete-time Langevin splitting methods into agreement with thermodynamics. Journal of Chemical Physics, 2021, 155, 184104.	3.0	3