

# J Alfredo Freites

## List of Publications by Year in descending order

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70  
papers

5,530  
citations

304368

22  
h-index

155451

55  
g-index

70  
all docs

70  
docs citations

70  
times ranked

7265  
citing authors

#	ARTICLE	IF	CITATIONS
1	Thermodynamics and Mechanism of the Membrane Permeation of Hv1 Channel Blockers. <i>Journal of Membrane Biology</i> , 2021, 254, 5-16.	1.0	6
2	Effects of Cardiolipin on the Conformational Dynamics of Membrane-Anchored Bcl-xL. <i>International Journal of Molecular Sciences</i> , 2021, 22, 9388.	1.8	4
3	Anomalous Diffusion of Peripheral Membrane Signaling Proteins from All-Atom Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2021, 125, 9990-9998.	1.2	1
4	Human $\beta$ -crystallin discriminates between aggregation-prone and function-preserving variants of a client protein. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2020, 1864, 129502.	1.1	7
5	Insights on small molecule binding to the Hv1 proton channel from free energy calculations with molecular dynamics simulations. <i>Scientific Reports</i> , 2020, 10, 13587.	1.6	8
6	Voltage-dependent structural models of the human Hv1 proton channel from long-timescale molecular dynamics simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 13490-13498.	3.3	29
7	Molecular Mechanism of Aggregation of the Cataract-Related $\beta$ -Crystallin W42R Variant from Multiscale Atomistic Simulations. <i>Biochemistry</i> , 2019, 58, 3691-3699.	1.2	16
8	Voltage-Dependent Profile Structures of a Kv-Channel via Time-Resolved Neutron Interferometry. <i>Biophysical Journal</i> , 2019, 117, 751-766.	0.2	3
9	Computational Insights on Small Molecule Binding to the Hv1 Proton Channel. <i>Biophysical Journal</i> , 2019, 116, 432a.	0.2	0
10	Experimental and Simulation Studies of Aquaporin 0 Water Permeability and Regulation. <i>Chemical Reviews</i> , 2019, 119, 6015-6039.	23.0	25
11	Cooperativity and allostery in aquaporin 0 regulation by Ca <sup>2+</sup> . <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2019, 1861, 988-996.	1.4	16
12	Role of Conformational Flexibility in Monte Carlo Simulations of Many-Protein Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1399-1408.	2.3	6
13	Molecular Arrangement of a Mixture of Organosulfur Surfactants at the Aqueous Solution-Vapor Interface Studied by Photoelectron Intensity and Angular Distribution Measurements and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2019, 123, 8160-8170.	1.5	11
14	Refining Protein Penetration into the Lipid Bilayer Using Fluorescence Quenching and Molecular Dynamics Simulations: The Case of Diphtheria Toxin Translocation Domain. <i>Journal of Membrane Biology</i> , 2018, 251, 379-391.	1.0	18
15	Calmodulin Gates Aquaporin 0 Permeability through a Positively Charged Cytoplasmic Loop. <i>Journal of Biological Chemistry</i> , 2017, 292, 185-195.	1.6	26
16	Atomistic Modeling of Ion Conduction through the Voltage-Sensing Domain of the <i>Shaker</i> K <sup>+</sup> Ion Channel. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3804-3812.	1.2	9
17	Gating energetics of a voltage-dependent K <sup>+</sup> channel pore domain. <i>Journal of Computational Chemistry</i> , 2017, 38, 1472-1478.	1.5	4
18	Transmembrane helices containing a charged arginine are thermodynamically stable. <i>European Biophysics Journal</i> , 2017, 46, 627-637.	1.2	21

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19	Specific cation effects at aqueous solution <sup>+</sup> vapor interfaces: Surfactant-like behavior of Li <sup>+</sup> revealed by experiments and simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 13363-13368.	3.3	34
20	YidC Insertase of <i>Escherichia coli</i> : Water Accessibility and Membrane Shaping. <i>Structure</i> , 2017, 25, 1403-1414.e3.	1.6	50
21	Two transmembrane dimers of the bovine papillomavirus E5 oncoprotein clamp the PDGF $\beta$ receptor in an active dimeric conformation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E7262-E7271.	3.3	26
22	Multi-Microsecond Molecular Dynamics Simulations of the HV1 Proton Channel. <i>Biophysical Journal</i> , 2016, 110, 282a-283a.	0.2	0
23	An Arginine-Rich Loop is Critical for the Modulation of the Water Permeability of Aquaporin 0. <i>Biophysical Journal</i> , 2016, 110, 382a-383a.	0.2	0
24	Multi-Conformation Monte Carlo: A Method for Introducing Flexibility in Efficient Simulations of Many-Protein Systems. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8115-8126.	1.2	12
25	Sequence comparison, molecular modeling, and network analysis predict structural diversity in cysteine proteases from the Cape sundew, <i>Drosera capensis</i> . <i>Computational and Structural Biotechnology Journal</i> , 2016, 14, 271-282.	1.9	19
26	Modeling Interprotein Interactions in Concentrated Solutions of Wild-Type and Cataract-Related Variants of $\beta$ - and $\gamma$ -Crystallins. <i>Biophysical Journal</i> , 2016, 110, 386a.	0.2	0
27	Computational Study of Anthracycline Interactions with Membrane-Embedded P-Glycoprotein. <i>Biophysical Journal</i> , 2016, 110, 57a.	0.2	0
28	Interleaflet mixing and coupling in liquid-disordered phospholipid bilayers. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 354-362.	1.4	29
29	Increased hydrophobic surface exposure in the cataract-related G18V variant of human $\beta$ -crystallin. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2016, 1860, 325-332.	1.1	20
30	Introducing Molecular Flexibility in Efficient Simulations of Many-Protein Systems. <i>Biophysical Journal</i> , 2015, 108, 470a.	0.2	0
31	Voltage Sensing in Membranes: From Macroscopic Currents to Molecular Motions. <i>Journal of Membrane Biology</i> , 2015, 248, 419-430.	1.0	18
32	Molecular Biophysics of Orai Store-Operated Ca <sup>2+</sup> Channels. <i>Biophysical Journal</i> , 2015, 108, 237-246.	0.2	64
33	Specific ion interactions with aromatic rings in aqueous solutions: Comparison of molecular dynamics simulations with a thermodynamic solute partitioning model and Raman spectroscopy. <i>Chemical Physics Letters</i> , 2015, 638, 1-8.	1.2	6
34	Structural Plasticity in the Topology of the Membrane-Interacting Domain of HIV-1 gp41. <i>Biophysical Journal</i> , 2014, 106, 610-620.	0.2	22
35	Direct Evidence of Conformational Changes Associated with Voltage Gating in a Voltage Sensor Protein by Time-Resolved X-ray/Neutron Interferometry. <i>Langmuir</i> , 2014, 30, 4784-4796.	1.6	16
36	Atomistic Molecular Dynamics Simulations of <i>Drosophila</i> Orai in a Hydrated Lipid Bilayer. <i>Biophysical Journal</i> , 2014, 106, 316a.	0.2	1

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37	Atomistic Modeling of Ion Conduction through Voltage-Sensing Domains. <i>Biophysical Journal</i> , 2014, 106, 538a.	0.2	0
38	Molecular Dynamics Simulation Studies of Ion Permeation Pathways and Energetics in the Hv1 Proton Channel. <i>Biophysical Journal</i> , 2013, 104, 276a.	0.2	0
39	Allosteric mechanism of water-channel gating by Ca <sup>2+</sup> -calmodulin. <i>Nature Structural and Molecular Biology</i> , 2013, 20, 1085-1092.	3.6	102
40	Molecular Dynamics Simulations of Gammas-Crystallin. <i>Biophysical Journal</i> , 2013, 104, 46a.	0.2	0
41	Voltage-Gating in the Hv1 Proton Channel: Clues from Atomistic Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2012, 102, 686a.	0.2	0
42	Structural Characterization of the Voltage-Sensor Domain and Voltage-Gated K <sup>+</sup> -Channel Proteins Vectorially Oriented within a Single Bilayer Membrane at the Solid/Vapor and Solid/Liquid Interfaces via Neutron Interferometry. <i>Langmuir</i> , 2012, 28, 10504-10520.	1.6	14
43	Interaction of Water Vapor with the Surfaces of Imidazolium-Based Ionic Liquid Nanoparticles and Thin Films. <i>Journal of Physical Chemistry B</i> , 2012, 116, 11255-11265.	1.2	18
44	Outer membrane phospholipase A in phospholipid bilayers: A model system for concerted computational and experimental investigations of amino acid side chain partitioning into lipid bilayers. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2012, 1818, 126-134.	1.4	39
45	Water wires in atomistic models of the Hv1 proton channel. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2012, 1818, 286-293.	1.4	67
46	Coupling between the voltage-sensing and pore domains in a voltage-gated potassium channel. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2012, 1818, 1726-1736.	1.4	18
47	Assembly and stability of $\alpha$ -helical membrane proteins. <i>Soft Matter</i> , 2012, 8, 7742.	1.2	28
48	Microscopic Origin of Gating Current Fluctuations in a Potassium Channel Voltage Sensor. <i>Biophysical Journal</i> , 2012, 102, L44-L46.	0.2	28
49	Proton-Coupled Dynamics in Lactose Permease. <i>Structure</i> , 2012, 20, 1893-1904.	1.6	53
50	Microscopic Origin of Gating Current Fluctuations in a Potassium Channel Voltage Sensor. <i>Biophysical Journal</i> , 2012, 102, 686a.	0.2	0
51	Structural Dynamics of the S4 Voltage-Sensor Helix in Lipid Bilayers Lacking Phosphate Groups. <i>Journal of Physical Chemistry B</i> , 2011, 115, 8732-8738.	1.2	18
52	A potassium Channel Voltage-Sensing Domain in a Non-Phospholipid Bilayer. <i>Biophysical Journal</i> , 2011, 100, 282a.	0.2	0
53	Separating Instability from Aggregation Propensity in $\hat{I}^3$ S-Crystallin Variants. <i>Biophysical Journal</i> , 2011, 100, 498-506.	0.2	64
54	Proton Conduction via Water Wire in the Hv1 Proton Channel. <i>Biophysical Journal</i> , 2011, 100, 131a.	0.2	0

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55	Acyl-Chain Methyl Distributions of Liquid-Ordered and -Disordered Membranes. <i>Biophysical Journal</i> , 2011, 100, 1455-1462.	0.2	70
56	Arginine in Membranes: The Connection Between Molecular Dynamics Simulations and Translocon-Mediated Insertion Experiments. <i>Journal of Membrane Biology</i> , 2011, 239, 35-48.	1.0	104
57	Update of the CHARMM All-Atom Additive Force Field for Lipids: Validation on Six Lipid Types. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7830-7843.	1.2	3,676
58	Dynamics of SecY Translocons with Translocation-Defective Mutations. <i>Structure</i> , 2010, 18, 847-857.	1.6	47
59	Neutron Scattering and MD Simulation Study of DOPC and DOPC/cholesterol Bilayers. <i>Biophysical Journal</i> , 2010, 98, 493a.	0.2	0
60	Structure of a DOTAP Lipid Bilayer: A Concerted Neutron Scattering and Molecular Dynamics Study. <i>Biophysical Journal</i> , 2010, 98, 492a.	0.2	1
61	Down-State Model of the Voltage-Sensing Domain of a Potassium Channel. <i>Biophysical Journal</i> , 2010, 98, 2857-2866.	0.2	33
62	Down-State Model of the KvAP Full Channel. <i>Biophysical Journal</i> , 2010, 98, 315a.	0.2	1
63	Structure and hydration of membranes embedded with voltage-sensing domains. <i>Nature</i> , 2009, 462, 473-479.	13.7	175
64	Down-State Model of the KvAP Voltage-Sensing Domain. <i>Biophysical Journal</i> , 2009, 96, 484a.	0.2	0
65	Opening and closing of the periplasmic gate in lactose permease. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 3774-3778.	3.3	84
66	A Voltage-Sensor Water Pore. <i>Biophysical Journal</i> , 2006, 91, L90-L92.	0.2	89
67	Interface connections of a transmembrane voltage sensor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 15059-15064.	3.3	208
68	Annexin A1 Interaction with a Zwitterionic Phospholipid Monolayer: A Fluorescence Microscopy Study. <i>Langmuir</i> , 2004, 20, 11674-11683.	1.6	22
69	Molecular Dynamics Simulations of a Pulmonary Surfactant Protein B Peptide in a Lipid Monolayer. <i>Biophysical Journal</i> , 2003, 84, 2169-2180.	0.2	36
70	Synthesis and characterization of nanophase particles obtained by D.C. sputtering. <i>Scripta Materialia</i> , 2001, 44, 1883-1887.	2.6	8