Igor V Vorobyov

List of Publications by Year
in descending order

52	12,142	159585	243625
papers	citations	30 h-index	44 g-index

59	59	59	14376
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	CHARMM general force field: A force field for drugâ€like molecules compatible with the CHARMM allâ€atom additive biological force fields. Journal of Computational Chemistry, 2010, 31, 671-690.	3.3	4,718
2	Update of the CHARMM All-Atom Additive Force Field for Lipids: Validation on Six Lipid Types. Journal of Physical Chemistry B, 2010, 114, 7830-7843.	2.6	3,676
3	A polarizable model of water for molecular dynamics simulations of biomolecules. Chemical Physics Letters, 2006, 418, 245-249.	2.6	548
4	Simulating Monovalent and Divalent Ions in Aqueous Solution Using a Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2010, 6, 774-786.	5.3	401
5	Determination of Electrostatic Parameters for a Polarizable Force Field Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2005, 1, 153-168.	5.3	260
6	The Different Interactions of Lysine and Arginine Side Chains with Lipid Membranes. Journal of Physical Chemistry B, 2013, 117, 11906-11920.	2.6	245
7	Additive and Classical Drude Polarizable Force Fields for Linear and Cyclic Ethers. Journal of Chemical Theory and Computation, 2007, 3, 1120-1133.	5.3	233
8	Polarizable Empirical Force Field for Alkanes Based on the Classical Drude Oscillator Model. Journal of Physical Chemistry B, 2005, 109, 18988-18999.	2.6	193
9	Atomic Level Anisotropy in the Electrostatic Modeling of Lone Pairs for a Polarizable Force Field Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2006, 2, 1587-1597.	5.3	142
10	Polarizable Empirical Force Field for the Primary and Secondary Alcohol Series Based on the Classical Drude Model. Journal of Chemical Theory and Computation, 2007, 3, 1927-1946.	5.3	136
11	Potential of Mean Force and pK_a Profile Calculation for a Lipid Membrane-Exposed Arginine Side Chain. Journal of Physical Chemistry B, 2008, 112, 9574-9587.	2.6	107
12	Assessing Atomistic and Coarse-Grained Force Fields for Proteinâ^'Lipid Interactions: the Formidable Challenge of an Ionizable Side Chain in a Membrane. Journal of Physical Chemistry B, 2008, 112, 9588-9602.	2.6	103
13	Ion conduction and conformational flexibility of a bacterial voltage-gated sodium channel. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 3454-3459.	7.1	95
14	Ion-Induced Defect Permeation of Lipid Membranes. Biophysical Journal, 2014, 106, 586-597.	0.5	93
15	Hydrogen Bonding in Monomers and Dimers of 2-Aminoethanol. Journal of Physical Chemistry A, 2002, 106, 668-679.	2.5	89
16	Local anesthetic and antiepileptic drug access and binding to a bacterial voltage-gated sodium channel. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 13057-13062.	7.1	87
17	Atomistic Simulations of Membrane Ion Channel Conduction, Gating, and Modulation. Chemical Reviews, 2019, 119, 7737-7832.	47.7	87
18	Conformational studies of sphingolipids by NMR spectroscopy. II. Sphingomyelin. Biochimica Et Biophysica Acta - Biomembranes, 2000, 1467, 326-337.	2.6	86

#	Article	IF	Citations
19	Is Arginine Charged in a Membrane?. Biophysical Journal, 2008, 94, L11-L13.	0.5	81
20	Glycero- versus sphingo-phospholipids: correlations with human and non-human mammalian lens growth. Experimental Eye Research, 2003, 76, 725-734.	2.6	80
21	Structural basis for antiarrhythmic drug interactions with the human cardiac sodium channel. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 2945-2954.	7.1	71
22	The role of membrane thickness in charged proteinâ€“lipid interactions. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 135-145.	2.6	66
23	A Computational Pipeline to Predict Cardiotoxicity. Circulation Research, 2020, 126, 947-964.	4.5	60
24	Electrostatics of Deformable Lipid Membranes. Biophysical Journal, 2010, 98, 2904-2913.	0.5	49
25	The Role of Atomic Polarization in the Thermodynamics of Chloroform Partitioning to Lipid Bilayers. Journal of Chemical Theory and Computation, 2012, 8, 618-628.	5.3	47
26	On the role of anionic lipids in charged protein interactions with membranes. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 1673-1683.	2.6	44
27	Exploring the free-energy landscape of GPCR activation. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10327-10332.	7.1	43
28	A multiscale computational modelling approach predicts mechanisms of female sex risk in the setting of arousalâ€induced arrhythmias. Journal of Physiology, 2017, 595, 4695-4723.	2.9	41
29	The electrostatics of solvent and membrane interfaces and the role of electronic polarizability. Journal of Chemical Physics, 2010, 132, 185101.	3.0	38
30	Refining the treatment of membrane proteins by coarseâ€grained models. Proteins: Structure, Function and Bioinformatics, 2016, 84, 92-117.	2.6	37
31	Selectivity filter modalities and rapid inactivation of the hERG1 channel. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 2795-2804.	7.1	31
32	Challenges and advances in atomistic simulations of potassium and sodium ion channel gating and permeation. Journal of Physiology, 2019, 597, 679-698.	2.9	30
33	Energetic and Topological Analyses of Cooperative ÏƒH- and Ï€H-Bonding Interactions. Journal of Physical Chemistry A, 2002, 106, 10691-10699.	2.5	24
34	Digging into Lipid Membrane Permeation for Cardiac Ion Channel Blocker d-Sotalol with All-Atom Simulations. Frontiers in Pharmacology, 2018, 9, 26.	3.5	24
35	Rearrangement of a unique Kv1.3 selectivity filter conformation upon binding of a drug. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	20
36	A deep learning algorithm to translate and classify cardiac electrophysiology. ELife, 2021, 10, .	6.0	14

#	Article	IF	Citations
37	Molecular Dynamics Simulations Based on Polarizable Models Show that Ion Permeation Interconverts between Different Mechanisms as a Function of Membrane Thickness. Journal of Physical Chemistry B, 2021, 125, 1020-1035.	2.6	12
38	Molecular determinants of pro-arrhythmia proclivity of d- and l-sotalol via a multi-scale modeling pipeline. Journal of Molecular and Cellular Cardiology, 2021, 158, 163-177.	1.9	10
39	Orbital interactions in stable and metastable conformations of the dimethylphosphate anion. Computational and Theoretical Chemistry, 2001, 544, 91-109.	1.5	6
40	A demonstration of modularity, reuse, reproducibility, portability and scalability for modeling and simulation of cardiac electrophysiology using Kepler Workflows. PLoS Computational Biology, 2019, 15, e1006856.	3.2	4
41	Sex, drugs, and funky rhythms. Heart Rhythm, 2018, 15, 485-486.	0.7	3
42	Chapter 15 Charged Protein Side Chain Movement in Lipid Bilayers Explored with Free Energy Simulation. Current Topics in Membranes, 2008, , 405-459.	0.9	2
43	Structural Modeling of Local Anesthetic and Antiarrhythmic Drug Binding to the Human Cardiac Voltage Gated Sodium Channel. Biophysical Journal, 2018, 114, 39a.	0.5	2
44	Long Molecular Dynamics Simulations of the Voltage-Gated Sodium Channel, NavAb. Biophysical Journal, 2013, 104, 137a.	0.5	1
45	On the Roles of Anionic Lipids in Protein Localization and Permeability of Membranes. Biophysical Journal, 2010, 98, 81a-82a.	0.5	0
46	Origins of Non-Selective Ion Transport across Lipid Bilayers. Biophysical Journal, 2012, 102, 335a.	0.5	0
47	Effect of Lipid Unsaturation on Membrane Protein Structure and Function from Multi-Microsecond Molecular Dynamics Simulations. Biophysical Journal, 2012, 102, 498a.	0.5	0
48	The Distributions and Orientations of Retinoids in Retinal Membranes Studied with All-Atom Molecular Dynamics Simulations. Biophysical Journal, 2014, 106, 499a.	0.5	0
49	The Origins of Ion Selectivity in a Bacterial Sodium Channel Revealed by Î¼S-Long Simulations. Biophysical Journal, 2014, 106, 131a.	0.5	0
50	Charged Protein-Lipid Interactions in Bilayers with Wide-Ranging Thickness. Biophysical Journal, 2014, 106, 98a.	0.5	0
51	Uncovering the Links Between Conformational Flexibility and Function for a Bacterial Voltage-Gated Sodium Channel. Biophysical Journal, 2014, 106, 130a.	0.5	0
52	A mechanism underlying hERG current increase by a blocker. Proceedings for Annual Meeting of the Japanese Pharmacological Society, 2021, 94, 3-O-D2-1.	0.0	0