

Igor V Vorobyov

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/4677973/publications.pdf>

Version: 2024-02-01

52
papers

12,142
citations

182225

30
h-index

274796

44
g-index

59
all docs

59
docs citations

59
times ranked

16244
citing authors

#	ARTICLE	IF	CITATIONS
1	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, .	3.3	20
2	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.	1.2	12
3	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
4	A deep learning algorithm to translate and classify cardiac electrophysiology. ELife, 2021, 10, .	2.8	14
5	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.	0.9	10
6	A Computational Pipeline to Predict Cardiotoxicity. Circulation Research, 2020, 126, 947-964.	2.0	60
7	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.	3.3	31
8	Atomistic Simulations of Membrane Ion Channel Conduction, Gating, and Modulation. Chemical Reviews, 2019, 119, 7737-7832.	23.0	87
9	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.	1.5	4
10	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.	3.3	71
11	Challenges and advances in atomistic simulations of potassium and sodium ion channel gating and permeation. Journal of Physiology, 2019, 597, 679-698.	1.3	30
12	Sex, drugs, and funky rhythms. Heart Rhythm, 2018, 15, 485-486.	0.3	3
13	Structural Modeling of Local Anesthetic and Antiarrhythmic Drug Binding to the Human Cardiac Voltage Gated Sodium Channel. Biophysical Journal, 2018, 114, 39a.	0.2	2
14	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.	3.3	43
15	Digging into Lipid Membrane Permeation for Cardiac Ion Channel Blocker d-Sotalol with All-Atom Simulations. Frontiers in Pharmacology, 2018, 9, 26.	1.6	24
16	A multiscale computational modelling approach predicts mechanisms of female sex risk in the setting of arousal-induced arrhythmias. Journal of Physiology, 2017, 595, 4695-4723.	1.3	41
17	Refining the treatment of membrane proteins by coarse-grained models. Proteins: Structure, Function and Bioinformatics, 2016, 84, 92-117.	1.5	37
18	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.	3.3	95

#	ARTICLE	IF	CITATIONS
19	The Distributions and Orientations of Retinoids in Retinal Membranes Studied with All-Atom Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2014, 106, 499a.	0.2	0
20	Ion-Induced Defect Permeation of Lipid Membranes. <i>Biophysical Journal</i> , 2014, 106, 586-597.	0.2	93
21	Local anesthetic and antiepileptic drug access and binding to a bacterial voltage-gated sodium channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 13057-13062.	3.3	87
22	The Origins of Ion Selectivity in a Bacterial Sodium Channel Revealed by 1/4S-Long Simulations. <i>Biophysical Journal</i> , 2014, 106, 131a.	0.2	0
23	Charged Protein-Lipid Interactions in Bilayers with Wide-Ranging Thickness. <i>Biophysical Journal</i> , 2014, 106, 98a.	0.2	0
24	Uncovering the Links Between Conformational Flexibility and Function for a Bacterial Voltage-Gated Sodium Channel. <i>Biophysical Journal</i> , 2014, 106, 130a.	0.2	0
25	The Different Interactions of Lysine and Arginine Side Chains with Lipid Membranes. <i>Journal of Physical Chemistry B</i> , 2013, 117, 11906-11920.	1.2	245
26	Long Molecular Dynamics Simulations of the Voltage-Gated Sodium Channel, NavAb. <i>Biophysical Journal</i> , 2013, 104, 137a.	0.2	1
27	Origins of Non-Selective Ion Transport across Lipid Bilayers. <i>Biophysical Journal</i> , 2012, 102, 335a.	0.2	0
28	The role of membrane thickness in charged protein-lipid interactions. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2012, 1818, 135-145.	1.4	66
29	The Role of Atomic Polarization in the Thermodynamics of Chloroform Partitioning to Lipid Bilayers. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 618-628.	2.3	47
30	Effect of Lipid Unsaturation on Membrane Protein Structure and Function from Multi-Microsecond Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2012, 102, 498a.	0.2	0
31	On the role of anionic lipids in charged protein interactions with membranes. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2011, 1808, 1673-1683.	1.4	44
32	CHARMM general force field: A force field for drug-like molecules compatible with the CHARMM all-atom additive biological force fields. <i>Journal of Computational Chemistry</i> , 2010, 31, 671-690.	1.5	4,718
33	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
34	The electrostatics of solvent and membrane interfaces and the role of electronic polarizability. <i>Journal of Chemical Physics</i> , 2010, 132, 185101.	1.2	38
35	On the Roles of Anionic Lipids in Protein Localization and Permeability of Membranes. <i>Biophysical Journal</i> , 2010, 98, 81a-82a.	0.2	0
36	Electrostatics of Deformable Lipid Membranes. <i>Biophysical Journal</i> , 2010, 98, 2904-2913.	0.2	49

#	ARTICLE	IF	CITATIONS
37	Simulating Monovalent and Divalent Ions in Aqueous Solution Using a Drude Polarizable Force Field. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 774-786.	2.3	401
38	Assessing Atomistic and Coarse-Grained Force Fields for Protein~Lipid Interactions: the Formidable Challenge of an Ionizable Side Chain in a Membrane. <i>Journal of Physical Chemistry B</i> , 2008, 112, 9588-9602.	1.2	103
39	Potential of Mean Force and pK _a Profile Calculation for a Lipid Membrane-Exposed Arginine Side Chain. <i>Journal of Physical Chemistry B</i> , 2008, 112, 9574-9587.	1.2	107
40	Is Arginine Charged in a Membrane?. <i>Biophysical Journal</i> , 2008, 94, L11-L13.	0.2	81
41	Chapter 15 Charged Protein Side Chain Movement in Lipid Bilayers Explored with Free Energy Simulation. <i>Current Topics in Membranes</i> , 2008, , 405-459.	0.5	2
42	Additive and Classical Drude Polarizable Force Fields for Linear and Cyclic Ethers. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1120-1133.	2.3	233
43	Polarizable Empirical Force Field for the Primary and Secondary Alcohol Series Based on the Classical Drude Model. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1927-1946.	2.3	136
44	Atomic Level Anisotropy in the Electrostatic Modeling of Lone Pairs for a Polarizable Force Field Based on the Classical Drude Oscillator. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1587-1597.	2.3	142
45	A polarizable model of water for molecular dynamics simulations of biomolecules. <i>Chemical Physics Letters</i> , 2006, 418, 245-249.	1.2	548
46	Determination of Electrostatic Parameters for a Polarizable Force Field Based on the Classical Drude Oscillator. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 153-168.	2.3	260
47	Polarizable Empirical Force Field for Alkanes Based on the Classical Drude Oscillator Model. <i>Journal of Physical Chemistry B</i> , 2005, 109, 18988-18999.	1.2	193
48	Glycero- versus sphingo-phospholipids: correlations with human and non-human mammalian lens growth. <i>Experimental Eye Research</i> , 2003, 76, 725-734.	1.2	80
49	Energetic and Topological Analyses of Cooperative Ĥ and Ĥ-Bonding Interactions. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10691-10699.	1.1	24
50	Hydrogen Bonding in Monomers and Dimers of 2-Aminoethanol. <i>Journal of Physical Chemistry A</i> , 2002, 106, 668-679.	1.1	89
51	Orbital interactions in stable and metastable conformations of the dimethylphosphate anion. <i>Computational and Theoretical Chemistry</i> , 2001, 544, 91-109.	1.5	6
52	Conformational studies of sphingolipids by NMR spectroscopy. II. Sphingomyelin. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2000, 1467, 326-337.	1.4	86