

# Sergei Y Noskov

## List of Publications by Citations

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140  
papers

4,585  
citations

36  
h-index

62  
g-index

148  
ext. papers

5,283  
ext. citations

5.7  
avg, IF

5.78  
L-index

#	Paper	IF	Citations
140	Control of ion selectivity in potassium channels by electrostatic and dynamic properties of carbonyl ligands. <i>Nature</i> , <b>2004</b> , 431, 830-4	50.4	453
139	Molecular dynamics study of hydration in ethanol-water mixtures using a polarizable force field. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 6705-13	3.4	246
138	Ion permeation through the alpha-hemolysin channel: theoretical studies based on Brownian dynamics and Poisson-Nernst-Planck electrodiffusion theory. <i>Biophysical Journal</i> , <b>2004</b> , 87, 2299-309	2.9	163
137	Emerging Diversity in Lipid-Protein Interactions. <i>Chemical Reviews</i> , <b>2019</b> , 119, 5775-5848	68.1	163
136	Control of ion selectivity in LeuT: two Na <sup>+</sup> binding sites with two different mechanisms. <i>Journal of Molecular Biology</i> , <b>2008</b> , 377, 804-18	6.5	160
135	Importance of hydration and dynamics on the selectivity of the KcsA and NaK channels. <i>Journal of General Physiology</i> , <b>2007</b> , 129, 135-43	3.4	159
134	Ion selectivity in potassium channels. <i>Biophysical Chemistry</i> , <b>2006</b> , 124, 279-91	3.5	144
133	Ion selectivity in channels and transporters. <i>Journal of General Physiology</i> , <b>2011</b> , 137, 415-26	3.4	127
132	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> , <b>2006</b> , 2, 1587-97	6.4	123
131	Free energy decomposition of protein-protein interactions. <i>Biophysical Journal</i> , <b>2001</b> , 81, 737-50	2.9	97
130	Representation of Ion-Protein Interactions Using the Drude Polarizable Force-Field. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 9401-16	3.4	80
129	Ion-controlled conformational dynamics in the outward-open transition from an occluded state of LeuT. <i>Biophysical Journal</i> , <b>2012</b> , 103, 878-88	2.9	77
128	Identification of novel cholesterol-binding regions in Kir2 channels. <i>Journal of Biological Chemistry</i> , <b>2013</b> , 288, 31154-64	5.4	77
127	Combined receptor and ligand-based approach to the universal pharmacophore model development for studies of drug blockade to the hERG1 pore domain. <i>Journal of Chemical Information and Modeling</i> , <b>2011</b> , 51, 463-74	6.1	77
126	Evidence for a third sodium-binding site in glutamate transporters suggests an ion/substrate coupling model. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2010</b> , 107, 13912-7	11.5	69
125	Two mechanisms of ion selectivity in protein binding sites. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2010</b> , 107, 20329-34	11.5	69
124	Modeling of open, closed, and open-inactivated states of the hERG1 channel: structural mechanisms of the state-dependent drug binding. <i>Journal of Chemical Information and Modeling</i> , <b>2012</b> , 52, 2760-74	6.1	60

123	A three-dimensional model of a group II intron RNA and its interaction with the intron-encoded reverse transcriptase. <i>Molecular Cell</i> , <b>2008</b> , 30, 472-85	17.6	60
122	Hydrophobic plug functions as a gate in voltage-gated proton channels. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2014</b> , 111, E273-82	11.5	59
121	Molecular mechanism of ion-ion and ion-substrate coupling in the Na <sup>+</sup> -dependent leucine transporter LeuT. <i>Biophysical Journal</i> , <b>2008</b> , 95, 4613-21	2.9	52
120	Potassium channels in the heart: structure, function and regulation. <i>Journal of Physiology</i> , <b>2017</b> , 595, 2209-2228	3.9	49
119	Current state of theoretical and experimental studies of the voltage-dependent anion channel (VDAC). <i>Biochimica Et Biophysica Acta - Biomembranes</i> , <b>2016</b> , 1858, 1778-90	3.8	49
118	The role of local hydration and hydrogen-bonding dynamics in ion and solute release from ion-coupled secondary transporters. <i>Biochemistry</i> , <b>2011</b> , 50, 1848-56	3.2	47
117	Sodium channel selectivity and conduction: prokaryotes have devised their own molecular strategy. <i>Journal of General Physiology</i> , <b>2014</b> , 143, 157-71	3.4	46
116	Ivabradine prolongs phase 3 of cardiac repolarization and blocks the hERG1 (KCNH2) current over a concentration-range overlapping with that required to block HCN4. <i>Journal of Molecular and Cellular Cardiology</i> , <b>2015</b> , 85, 71-8	5.8	46
115	ATP transport through VDAC and the VDAC-tubulin complex probed by equilibrium and nonequilibrium MD simulations. <i>Biochemistry</i> , <b>2013</b> , 52, 9246-56	3.2	45
114	Relative Free Energies for Hydration of Monovalent Ions from QM and QM/MM Simulations. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 4165-75	6.4	45
113	Insights into the molecular mechanism of hERG1 channel activation and blockade by drugs. <i>Current Medicinal Chemistry</i> , <b>2010</b> , 17, 3514-32	4.3	45
112	The molecular mechanism of ion-dependent gating in secondary transporters. <i>PLoS Computational Biology</i> , <b>2013</b> , 9, e1003296	5	44
111	Structural refinement of the hERG1 pore and voltage-sensing domains with ROSETTA-membrane and molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2010</b> , 78, 2922-34	4.2	44
110	The Role of Atomic Polarization in the Thermodynamics of Chloroform Partitioning to Lipid Bilayers. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 618-28	6.4	42
109	The RCK2 domain uses a coordination site present in Kir channels to confer sodium sensitivity to Slo2.2 channels. <i>Journal of Neuroscience</i> , <b>2010</b> , 30, 7554-62	6.6	42
108	Mechanism of the Association between Na <sup>+</sup> Binding and Conformations at the Intracellular Gate in Neurotransmitter:Sodium Symporters. <i>Journal of Biological Chemistry</i> , <b>2015</b> , 290, 13992-4003	5.4	41
107	4-(4-(dimethylamino)phenyl)-1-methylpyridinium (APP <sup>+</sup> ) is a fluorescent substrate for the human serotonin transporter. <i>Journal of Biological Chemistry</i> , <b>2012</b> , 287, 8852-63	5.4	38
106	A human ether-à-go-go-related (hERG) ion channel atomistic model generated by long supercomputer molecular dynamics simulations and its use in predicting drug cardiotoxicity. <i>Toxicology Letters</i> , <b>2014</b> , 230, 382-92	4.4	37

105	Quantum effects in cation interactions with first and second coordination shell ligands in metalloproteins. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 4992-5001	6.4	36
104	Acidification asymmetrically affects voltage-dependent anion channel implicating the involvement of salt bridges. <i>Journal of Biological Chemistry</i> , <b>2014</b> , 289, 23670-82	5.4	36
103	The structural pathway for water permeation through sodium-glucose cotransporters. <i>Biophysical Journal</i> , <b>2011</b> , 101, 1887-95	2.9	35
102	Interactions of H562 in the S5 helix with T618 and S621 in the pore helix are important determinants of hERG1 potassium channel structure and function. <i>Biophysical Journal</i> , <b>2009</b> , 96, 3600-10 <sup>2-9</sup>	2.9	35
101	Pendular proteins in gases and new avenues for characterization of macromolecules by ion mobility spectrometry. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2009</b> , 106, 6495-500	11.5	34
100	Hydration number, topological control, and ion selectivity. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 8725-30	3.4	34
99	Molecular mechanism of substrate specificity in the bacterial neutral amino acid transporter LeuT. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2008</b> , 73, 851-63	4.2	32
98	Cholesterol up-regulates neuronal G protein-gated inwardly rectifying potassium (GIRK) channel activity in the hippocampus. <i>Journal of Biological Chemistry</i> , <b>2017</b> , 292, 6135-6147	5.4	31
97	Magic angle spinning nuclear magnetic resonance characterization of voltage-dependent anion channel gating in two-dimensional lipid crystalline bilayers. <i>Biochemistry</i> , <b>2015</b> , 54, 994-1005	3.2	31
96	A conserved asparagine residue in transmembrane segment 1 (TM1) of serotonin transporter dictates chloride-coupled neurotransmitter transport. <i>Journal of Biological Chemistry</i> , <b>2011</b> , 286, 30823-30836	5.4	31
95	Structural features and lipid binding domain of tubulin on biomimetic mitochondrial membranes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2017</b> , 114, E3622-E3631	11.5	30
94	In silico prediction of drug therapy in catecholaminergic polymorphic ventricular tachycardia. <i>Journal of Physiology</i> , <b>2016</b> , 594, 567-93	3.9	28
93	Selective ion binding and transport by membrane proteins I: A computational perspective. <i>Coordination Chemistry Reviews</i> , <b>2017</b> , 345, 108-136	23.2	27
92	Elucidating factors important for monovalent cation selectivity in enzymes: E. coli $\beta$ -galactosidase as a model. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 10899-909	3.6	27
91	A Computational Pipeline to Predict Cardiotoxicity: From the Atom to the Rhythm. <i>Circulation Research</i> , <b>2020</b> , 126, 947-964	15.7	27
90	Molecular mechanism of Zn <sup>2+</sup> inhibition of a voltage-gated proton channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2016</b> , 113, E5962-E5971	11.5	26
89	Model of ionic currents through microtubule nanopores and the lumen. <i>Physical Review E</i> , <b>2010</b> , 81, 051912	12	26
88	Structure of methanol-methanol associates in dilute methanol-water mixtures from molecular dynamics simulation. <i>Journal of Molecular Liquids</i> , <b>2001</b> , 91, 157-165	6	26

87	Structure-guided topographic mapping and mutagenesis to elucidate binding sites for the human ether-a-go-go-related gene 1 potassium channel (KCNH2) activator NS1643. <i>Journal of Pharmacology and Experimental Therapeutics</i> , <b>2012</b> , 342, 441-52	4.7	25
86	A multiscale computational modelling approach predicts mechanisms of female sex risk in the setting of arousal-induced arrhythmias. <i>Journal of Physiology</i> , <b>2017</b> , 595, 4695-4723	3.9	24
85	BROMOC-D: Brownian Dynamics/Monte-Carlo Program Suite to Study Ion and DNA Permeation in Nanopores. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 2540-2551	6.4	24
84	A Guide to QM/MM Methodology and Applications. <i>Advances in Quantum Chemistry</i> , <b>2010</b> , 59, 353-400	1.4	24
83	Distant cytosolic residues mediate a two-way molecular switch that controls the modulation of inwardly rectifying potassium (Kir) channels by cholesterol and phosphatidylinositol 4,5-bisphosphate (PI(4,5)P(2)). <i>Journal of Biological Chemistry</i> , <b>2012</b> , 287, 40266-78	5.4	24
82	Improving the LIE Method for Binding Free Energy Calculations of Protein-Ligand Complexes. <i>Journal of Chemical Information and Modeling</i> , <b>2015</b> , 55, 1867-77	6.1	23
81	NS1643 interacts around L529 of hERG to alter voltage sensor movement on the path to activation. <i>Biophysical Journal</i> , <b>2015</b> , 108, 1400-1413	2.9	23
80	Evaluations of the Absolute and Relative Free Energies for Antidepressant Binding to the Amino Acid Membrane Transporter LeuT with Free Energy Simulations. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 1900-14	6.4	23
79	Mapping the gating and permeation pathways in the voltage-gated proton channel Hv1. <i>Journal of Molecular Biology</i> , <b>2015</b> , 427, 131-45	6.5	22
78	Performance of Machine Learning Algorithms for Qualitative and Quantitative Prediction Drug Blockade of hERG1 channel. <i>Computational Toxicology</i> , <b>2018</b> , 6, 55-63	3.1	22
77	Characterization of the Cation Binding Sites in the NCKX2 Na/Ca-K Exchanger. <i>Biochemistry</i> , <b>2016</b> , 55, 6445-6455	3.2	20
76	Role of the pH in state-dependent blockade of hERG currents. <i>Scientific Reports</i> , <b>2016</b> , 6, 32536	4.9	20
75	Atomistic models of ion and solute transport by the sodium-dependent secondary active transporters. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , <b>2012</b> , 1818, 337-47	3.8	20
74	Estimation of Potentials of Mean Force from Nonequilibrium Pulling Simulations Using Both Minh-Adib Estimator and Weighted Histogram Analysis Method. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 1000-10	6.4	19
73	Polarizable model of chloroform based on classical Drude oscillators. <i>Chemical Physics Letters</i> , <b>2009</b> , 468, 270-274	2.5	19
72	The QM-MM interface for CHARMM-deMon. <i>Journal of Computational Chemistry</i> , <b>2010</b> , 31, 1015-23	3.5	19
71	Kinetic model for NS1643 drug activation of WT and L529I variants of Kv11.1 (hERG1) potassium channel. <i>Biophysical Journal</i> , <b>2015</b> , 108, 1414-1424	2.9	18
70	Cholesterol sensitivity of KIR2.1 depends on functional inter-links between the N and C termini. <i>Channels</i> , <b>2013</b> , 7, 303-12	3	18

69	Selectivity filter modalities and rapid inactivation of the hERG1 channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2020</b> , 117, 2795-2804	11.5	17
68	Determinants of Isoform-Specific Gating Kinetics of hERG1 Channel: Combined Experimental and Simulation Study. <i>Frontiers in Physiology</i> , <b>2018</b> , 9, 207	4.6	17
67	Effect of confinement on DNA, solvent and counterion dynamics in a model biological nanopore. <i>Nanoscale</i> , <b>2014</b> , 6, 9006-16	7.7	17
66	The study of hydrophobic hydration in supercritical water-methanol mixtures. <i>Journal of Molecular Graphics and Modelling</i> , <b>2001</b> , 19, 412-6	2.8	17
65	LiCl solvation in N-methyl-acetamide (NMA) as a model for understanding Li(+) binding to an amide plane. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 4191-200	3.6	16
64	Atomistic models for free energy evaluation of drug binding to membrane proteins. <i>Current Medicinal Chemistry</i> , <b>2011</b> , 18, 2601-11	4.3	16
63	Comparative Analysis of Protein Hydration from MD simulations with Additive and Polarizable Force Fields. <i>Advanced Theory and Simulations</i> , <b>2019</b> , 2, 1800106	3.5	16
62	In silico investigation of PARP-1 catalytic domains in holo and apo states for the design of high-affinity PARP-1 inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2016</b> , 31, 112-20	5.6	15
61	The Pore-Lipid Interface: Role of Amino-Acid Determinants of Lipophilic Access by Ivabradine to the hERG1 Pore Domain. <i>Molecular Pharmacology</i> , <b>2019</b> , 96, 259-271	4.3	15
60	Microsecond simulations of DNA and ion transport in nanopores with novel ion-ion and ion-nucleotides effective potentials. <i>Journal of Computational Chemistry</i> , <b>2014</b> , 35, 711-21	3.5	15
59	Rehabilitating drug-induced long-QT promoters: in-silico design of hERG-neutral cisapride analogues with retained pharmacological activity. <i>BMC Pharmacology &amp; Toxicology</i> , <b>2014</b> , 15, 14	2.6	14
58	QM/MM calculations with deMon2k. <i>Molecules</i> , <b>2015</b> , 20, 4780-812	4.8	14
57	Structure driven design of novel human ether-a-go-go-related-gene channel (hERG1) activators. <i>PLoS ONE</i> , <b>2014</b> , 9, e105553	3.7	14
56	Molecular Simulations of Solved Co-crystallized X-Ray Structures Identify Action Mechanisms of PDE Inhibitors. <i>Biophysical Journal</i> , <b>2015</b> , 109, 1163-8	2.9	13
55	Digging into Lipid Membrane Permeation for Cardiac Ion Channel Blocker d-Sotalol with All-Atom Simulations. <i>Frontiers in Pharmacology</i> , <b>2018</b> , 9, 26	5.6	12
54	Electron Diffraction and Quantum Chemical Study of the Molecular Structure of para-Methylbenzenesulfonyl Fluoride and para-Methylbenzenesulfonyl Bromide. <i>Journal of Structural Chemistry</i> , <b>2000</b> , 41, 939-947	0.9	12
53	Molecular Mechanism of Conductance Enhancement in Narrow Cation-Selective Membrane Channels. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 3497-3502	6.4	11
52	Defective cell adhesion function of solute transporter, SLC4A11, in endothelial corneal dystrophies. <i>Human Molecular Genetics</i> , <b>2020</b> , 29, 97-116	5.6	10



51	Computational membrane biophysics: From ion channel interactions with drugs to cellular function. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , <b>2017</b> , 1865, 1643-1653	4	10
50	BROMOCEA Code: An Improved Grand Canonical Monte Carlo/Brownian Dynamics Algorithm Including Explicit Atoms. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 2401-17	6.4	10
49	Two-Dimensional Potentials of Mean Force of Nile Red in Intact and Damaged Model Bilayers. Application to Calculations of Fluorescence Spectra. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 364-71	6.4	9
48	Molecular strategies to achieve selective conductance in NaK channel variants. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 2041-9	3.4	9
47	Computational Models for Understanding of Structure, Function and Pharmacology of the Cardiac Potassium Channel Kv11.1 (hERG). <i>Current Topics in Medicinal Chemistry</i> , <b>2017</b> , 17, 2681-2702	3	9
46	K+ Block Is the Mechanism of Functional Asymmetry in Bacterial Na(v) Channels. <i>PLoS Computational Biology</i> , <b>2016</b> , 12, e1004482	5	9
45	What controls open-pore and residual currents in the first sensing zone of alpha-hemolysin nanopore? Combined experimental and theoretical study. <i>Nanoscale</i> , <b>2016</b> , 8, 11571-9	7.7	9
44	BROMOC suite: Monte Carlo/Brownian dynamics suite for studies of ion permeation and DNA transport in biological and artificial pores with effective potentials. <i>Journal of Computational Chemistry</i> , <b>2015</b> , 36, 264-71	3.5	8
43	Role of protein matrix rigidity and local polarization effects in the monovalent cation selectivity of crystallographic sites in the Na-coupled aspartate transporter Glt(Ph). <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 2397-404	3.6	8
42	SLC4A11 function: evidence for H(OH) and NH-H transport. <i>American Journal of Physiology - Cell Physiology</i> , <b>2020</b> , 318, C392-C405	5.4	8
41	Mapping Ryanodine Binding Sites in the Pore Cavity of Ryanodine Receptors. <i>Biophysical Journal</i> , <b>2017</b> , 112, 1645-1653	2.9	7
40	Inter-species variation in monovalent anion substrate selectivity and inhibitor sensitivity in the sodium iodide symporter (NIS). <i>PLoS ONE</i> , <b>2020</b> , 15, e0229085	3.7	7
39	Lipid roles in hERG function and interactions with drugs. <i>Neuroscience Letters</i> , <b>2019</b> , 700, 70-77	3.3	7
38	Long-Range Effects of Mutating R248 to Q/W in the p53 Core Domain. <i>Journal of Physical Chemistry B</i> , <b>2002</b> , 106, 13047-13057	3.4	7
37	Polarization Effects in Water-Mediated Selective Cation Transport across a Narrow Transmembrane Channel. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 1726-1741	6.4	7
36	Benchmarking polarizable and non-polarizable force fields for Ca-peptides against a comprehensive QM dataset. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 144102	3.9	5
35	Mapping of Ion and Substrate Binding Sites in Human Sodium Iodide Symporter (hNIS). <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 1652-1665	6.1	5
34	Mechanism of K+/Na+ selectivity in potassium channels from the perspective of the non-selective bacterial channel NaK. <i>Channels</i> , <b>2011</b> , 5, 198-200	3	5

33	Structure of voltage-dependent anion channel-tethered bilayer lipid membranes determined using neutron reflectivity. <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2018</b> , 74, 1219-1232	5.5	5
32	First universal pharmacophore model for hERG1 K channel activators: actHER. <i>Journal of Molecular Graphics and Modelling</i> , <b>2017</b> , 74, 153-170	2.8	4
31	Halothane solvation in water and organic solvents from molecular simulations with new polarizable potential function. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 6401-8	3.4	4
30	Na(+), K (+) and Tl(+) hydration from QM/MM computations and MD simulations with a polarizable force field. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , <b>2010</b> , 2, 12-20	3.5	4
29	Assessing hERG1 Blockade from Bayesian Machine-Learning-Optimized Site Identification by Ligand Competitive Saturation Simulations. <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 6489-6501	6.1	4
28	Allosteric Coupling Between Drug Binding and the Aromatic Cassette in the Pore Domain of the hERG1 Channel: Implications for a State-Dependent Blockade. <i>Frontiers in Pharmacology</i> , <b>2020</b> , 11, 914	5.6	4
27	Identification of PUFA interaction sites on the cardiac potassium channel KCNQ1. <i>Journal of General Physiology</i> , <b>2021</b> , 153,	3.4	4
26	Toward Reducing hERG Affinities for DAT Inhibitors with a Combined Machine Learning and Molecular Modeling Approach. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 4266-4279	6.1	4
25	Cryo-EM structure of the sodium-driven chloride/bicarbonate exchanger NDCBE. <i>Nature Communications</i> , <b>2021</b> , 12, 5690	17.4	4
24	Bases of Bacterial Sodium Channel Selectivity Among Organic Cations. <i>Scientific Reports</i> , <b>2019</b> , 9, 15260	4.9	3
23	Designing of multi-targeted molecules using combination of molecular screening and in silico drug cardiotoxicity prediction approaches. <i>Journal of Molecular Graphics and Modelling</i> , <b>2014</b> , 50, 16-34	2.8	3
22	VDAC Gating Thermodynamics, but Not Gating Kinetics, Are Virtually Temperature Independent. <i>Biophysical Journal</i> , <b>2020</b> , 119, 2584-2592	2.9	3
21	A molecular switch controls the impact of cholesterol on a Kir channel.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2022</b> , 119, e2109431119	11.5	3
20	Importance of hydration and dynamics on the selectivity of the KcsA and NaK channels. <i>Journal of General Physiology</i> , <b>2011</b> , 138, 651-651	3.4	2
19	Characterizing the Water Wire in the Gramicidin Channel Found by Monte Carlo Sampling Using Continuum Electrostatics and in Molecular Dynamics Trajectories with Conventional or Polarizable Force Fields. <i>Journal of Computational Biophysics and Chemistry</i> , <b>2021</b> , 20, 111-130		2
18	Atomistic modeling towards predictive cardiotoxicity		2
17	Lipid regulation of hERG1 channel function. <i>Nature Communications</i> , <b>2021</b> , 12, 1409	17.4	2
16	Refinement of a cryo-EM structure of hERG: Bridging structure and function. <i>Biophysical Journal</i> , <b>2021</b> , 120, 738-748	2.9	2



15	A second S4 movement opens hyperpolarization-activated HCN channels. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2021</b> , 118,	11.5	2
14	Identification of multiple substrate binding sites in SLC4 transporters in the outward-facing conformation: Insights into the transport mechanism. <i>Journal of Biological Chemistry</i> , <b>2021</b> , 296, 100724	5.4	2
13	Improved QM/MM Linear-Interaction Energy Model for Substrate Recognition in Zinc-Containing Metalloenzymes. <i>Journal of Physical Chemistry B</i> , <b>2016</b> , 120, 7824-35	3.4	1
12	Reply from Pei-Chi Yang, Jonathan D. Moreno, Mao-Tsuen Jeng, Xander H. T. Wehrens, Sergei Noskov and Colleen E. Clancy. <i>Journal of Physiology</i> , <b>2016</b> , 594, 6433-6435	3.9	1
11	Characterizing the water wire in the Gramicidin channel found by Monte Carlo sampling using continuum electrostatics and in molecular dynamics trajectories with conventional or polarizable force fields. <i>Journal of Theoretical and Computational Chemistry</i> , 2042001	1.8	1
10	C subunit of the ATP synthase is an amyloidogenic channel-forming peptide: possible implications in mitochondrial pathogenesis		1
9	Origin of the Phosphoprotein Phosphatase (PPP) sequence family in Bacteria: Critical ancestral sequence changes, radiation patterns and substrate binding features. <i>BBA Advances</i> , <b>2021</b> , 1, 100005		1
8	A general mechanism of KCNE1 modulation of KCNQ1 channels involving non-canonical VSD-PD coupling. <i>Communications Biology</i> , <b>2021</b> , 4, 887	6.7	0
7	Molecular determinants of pro-arrhythmia proclivity of d- and l-sotalol via a multi-scale modeling pipeline. <i>Journal of Molecular and Cellular Cardiology</i> , <b>2021</b> , 158, 163-177	5.8	0
6	In response to Melgari et al. "hERG potassium channel inhibition by ivabradine requires channel gating". <i>Journal of Molecular and Cellular Cardiology</i> , <b>2015</b> , 87, 192-3	5.8	
5	Nonequilibrium path-ensemble averages for symmetric protocols. <i>Journal of Chemical Physics</i> , <b>2019</b> , 151, 194103	3.9	
4	Inter-species variation in monovalent anion substrate selectivity and inhibitor sensitivity in the sodium iodide symporter (NIS) <b>2020</b> , 15, e0229085		
3	Inter-species variation in monovalent anion substrate selectivity and inhibitor sensitivity in the sodium iodide symporter (NIS) <b>2020</b> , 15, e0229085		
2	Inter-species variation in monovalent anion substrate selectivity and inhibitor sensitivity in the sodium iodide symporter (NIS) <b>2020</b> , 15, e0229085		
1	Inter-species variation in monovalent anion substrate selectivity and inhibitor sensitivity in the sodium iodide symporter (NIS) <b>2020</b> , 15, e0229085		