# Sergei Y Noskov

## List of Publications by Year in Descending Order



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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 | A molecular switch controls the impact of cholesterol on a Kir channel.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2109431119 | 11.5 | 3 |
| 139 | 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. *Journal of Computational Biophysics and Chemistry*, **2021**, 20, 111-130 | | 2 |
| 138 | Lipid regulation of hERG1 channel function. *Nature Communications*, **2021**, 12, 1409 | 17.4 | 2 |
| 137 | Identification of PUFA interaction sites on the cardiac potassium channel KCNQ1. *Journal of General Physiology*, **2021**, 153, | 3.4 | 4 |
| 136 | Polarization Effects in Water-Mediated Selective Cation Transport across a Narrow Transmembrane Channel. *Journal of Chemical Theory and Computation*, **2021**, 17, 1726-1741 | 6.4 | 7 |
| 135 | Refinement of a cryo-EM structure of hERG: Bridging structure and function. *Biophysical Journal*, **2021**, 120, 738-748 | 2.9 | 2 |
| 134 | A general mechanism of KCNE1 modulation of KCNQ1 channels involving non-canonical VSD-PD coupling. *Communications Biology*, **2021**, 4, 887 | 6.7 | 0 |
| 133 | Toward Reducing hERG Affinities for DAT Inhibitors with a Combined Machine Learning and Molecular Modeling Approach. *Journal of Chemical Information and Modeling*, **2021**, 61, 4266-4279 | 6.1 | 4 |
| 132 | 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 | 5.8 | 0 |
| 131 | A second S4 movement opens hyperpolarization-activated HCN channels. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118, | 11.5 | 2 |
| 130 | Cryo-EM structure of the sodium-driven chloride/bicarbonate exchanger NDCBE. *Nature Communications*, **2021**, 12, 5690 | 17.4 | 4 |
| 129 | Identification of multiple substrate binding sites in SLC4 transporters in the outward-facing conformation: Insights into the transport mechanism. *Journal of Biological Chemistry*, **2021**, 296, 100724 | 5.4 | 2 |
| 128 | Origin of the Phosphoprotein Phosphatase (PPP) sequence family in Bacteria: Critical ancestral sequence changes, radiation patterns and substrate binding features. *BBA Advances*, **2021**, 1, 100005 | | 1 |
| 127 | Benchmarking polarizable and non-polarizable force fields for Ca-peptides against a comprehensive QM dataset. *Journal of Chemical Physics*, **2020**, 153, 144102 | 3.9 | 5 |
| 126 | Mapping of Ion and Substrate Binding Sites in Human Sodium Iodide Symporter (hNIS). *Journal of Chemical Information and Modeling*, **2020**, 60, 1652-1665 | 6.1 | 5 |
| 125 | A Computational Pipeline to Predict Cardiotoxicity: From the Atom to the Rhythm. *Circulation Research*, **2020**, 126, 947-964 | 15.7 | 27 |
| 124 | Inter-species variation in monovalent anion substrate selectivity and inhibitor sensitivity in the sodium iodide symporter (NIS). *PLoS ONE*, **2020**, 15, e0229085 | 3.7 | 7 |

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| 123 | 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 | 11.5 | 17 |
| 122 | Defective cell adhesion function of solute transporter, SLC4A11, in endothelial corneal dystrophies. *Human Molecular Genetics*, **2020**, 29, 97-116 | 5.6 | 10 |
| 121 | SLC4A11 function: evidence for H(OH) and NH-H transport. *American Journal of Physiology - Cell Physiology*, **2020**, 318, C392-C405 | 5.4 | 8 |
| 120 | Assessing hERG1 Blockade from Bayesian Machine-Learning-Optimized Site Identification by Ligand Competitive Saturation Simulations. *Journal of Chemical Information and Modeling*, **2020**, 60, 6489-6501 | 6.1 | 4 |
| 119 | Allosteric Coupling Between Drug Binding and the Aromatic Cassette in the Pore Domain of the hERG1 Channel: Implications for a State-Dependent Blockade. *Frontiers in Pharmacology*, **2020**, 11, 914 | 5.6 | 4 |
| 118 | VDAC Gating Thermodynamics, but Not Gating Kinetics, Are Virtually Temperature Independent. *Biophysical Journal*, **2020**, 119, 2584-2592 | 2.9 | 3 |
| 117 | Inter-species variation in monovalent anion substrate selectivity and inhibitor sensitivity in the sodium iodide symporter (NIS) **2020**, 15, e0229085 | | |
| 116 | Inter-species variation in monovalent anion substrate selectivity and inhibitor sensitivity in the sodium iodide symporter (NIS) **2020**, 15, e0229085 | | |
| 115 | Inter-species variation in monovalent anion substrate selectivity and inhibitor sensitivity in the sodium iodide symporter (NIS) **2020**, 15, e0229085 | | |
| 114 | Inter-species variation in monovalent anion substrate selectivity and inhibitor sensitivity in the sodium iodide symporter (NIS) **2020**, 15, e0229085 | | |
| 113 | Lipid roles in hERG function and interactions with drugs. *Neuroscience Letters*, **2019**, 700, 70-77 | 3.3 | 7 |
| 112 | The Pore-Lipid Interface: Role of Amino-Acid Determinants of Lipophilic Access by Ivabradine to the hERG1 Pore Domain. *Molecular Pharmacology*, **2019**, 96, 259-271 | 4.3 | 15 |
| 111 | Bases of Bacterial Sodium Channel Selectivity Among Organic Cations. *Scientific Reports*, **2019**, 9, 15260 | 4.9 | 3 |
| 110 | Comparative Analysis of Protein Hydration from MD simulations with Additive and Polarizable Force Fields. *Advanced Theory and Simulations*, **2019**, 2, 1800106 | 3.5 | 16 |
| 109 | Emerging Diversity in Lipid-Protein Interactions. *Chemical Reviews*, **2019**, 119, 5775-5848 | 68.1 | 163 |
| 108 | Nonequilibrium path-ensemble averages for symmetric protocols. *Journal of Chemical Physics*, **2019** , 151, 194103 | 3.9 | |
| 107 | Performance of Machine Learning Algorithms for Qualitative and Quantitative Prediction Drug Blockade of hERG1 channel. *Computational Toxicology*, **2018**, 6, 55-63 | 3.1 | 22 |
| 106 | Digging into Lipid Membrane Permeation for Cardiac Ion Channel Blocker d-Sotalol with All-Atom Simulations. *Frontiers in Pharmacology*, **2018**, 9, 26 | 5.6 | 12 |

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| 105 | Determinants of Isoform-Specific Gating Kinetics of hERG1 Channel: Combined Experimental and Simulation Study. *Frontiers in Physiology*, **2018**, 9, 207 | 4.6 | 17 |
| 104 | Molecular Mechanism of Conductance Enhancement in Narrow Cation-Selective Membrane Channels. *Journal of Physical Chemistry Letters*, **2018**, 9, 3497-3502 | 6.4 | 11 |
| 103 | Structure of voltage-dependent anion channel-tethered bilayer lipid membranes determined using neutron reflectivity. *Acta Crystallographica Section D: Structural Biology*, **2018**, 74, 1219-1232 | 5.5 | 5 |
| 102 | Cholesterol up-regulates neuronal G protein-gated inwardly rectifying potassium (GIRK) channel activity in the hippocampus. *Journal of Biological Chemistry*, **2017**, 292, 6135-6147 | 5.4 | 31 |
| 101 | First universal pharmacophore model for hERG1 K channel activators: acthER. *Journal of Molecular Graphics and Modelling*, **2017**, 74, 153-170 | 2.8 | 4 |
| 100 | Structural features and lipid binding domain of tubulin on biomimetic mitochondrial membranes. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E3622-E3631 | 11.5 | 30 |
| 99 | Mapping Ryanodine Binding Sites in the Pore Cavity of Ryanodine Receptors. *Biophysical Journal*, **2017**, 112, 1645-1653 | 2.9 | 7 |
| 98 | 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 | 3.9 | 24 |
| 97 | Selective ion binding and transport by membrane proteins □A computational perspective. *Coordination Chemistry Reviews*, **2017**, 345, 108-136 | 23.2 | 27 |
| 96 | Computational membrane biophysics: From ion channel interactions with drugs to cellular function. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2017**, 1865, 1643-1653 | 4 | 10 |
| 95 | Potassium channels in the heart: structure, function and regulation. *Journal of Physiology*, **2017**, 595, 2209-2228 | 3.9 | 49 |
| 94 | Computational Models for Understanding of Structure, Function and Pharmacology of the Cardiac Potassium Channel Kv11.1 (hERG). *Current Topics in Medicinal Chemistry*, **2017**, 17, 2681-2702 | 3 | 9 |
| 93 | In silico investigation of PARP-1 catalytic domains in holo and apo states for the design of high-affinity PARP-1 inhibitors. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 112-20 | 5.6 | 15 |
| 92 | Characterization of the Cation Binding Sites in the NCKX2 Na/Ca-K Exchanger. *Biochemistry*, **2016**, 55, 6445-6455 | 3.2 | 20 |
| 91 | Molecular mechanism of Zn2+ inhibition of a voltage-gated proton channel. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E5962-E5971 | 11.5 | 26 |
| 90 | Improved QM/MM Linear-Interaction Energy Model for Substrate Recognition in Zinc-Containing Metalloenzymes. *Journal of Physical Chemistry B*, **2016**, 120, 7824-35 | 3.4 | 1 |
| 89 | Role of the pH in state-dependent blockade of hERG currents. *Scientific Reports*, **2016**, 6, 32536 | 4.9 | 20 |
| 88 | Reply from Pei-Chi Yang, Jonathan D. Moreno, Mao-Tsuen Jeng, Xander H. T. Wehrens, Sergei Noskov and Colleen E. Clancy. *Journal of Physiology*, **2016**, 594, 6433-6435 | 3.9 | 1 |

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| 87 | LiCl solvation in N-methyl-acetamide (NMA) as a model for understanding Li(+) binding to an amide plane. *Physical Chemistry Chemical Physics*, **2016**, 18, 4191-200 | 3.6 | 16 |
| 86 | Two-Dimensional Potentials of Mean Force of Nile Red in Intact and Damaged Model Bilayers. Application to Calculations of Fluorescence Spectra. *Journal of Chemical Theory and Computation*, **2016**, 12, 364-71 | 6.4 | 9 |
| 85 | Estimation of Potentials of Mean Force from Nonequilibrium Pulling Simulations Using Both Minh-Adib Estimator and Weighted Histogram Analysis Method. *Journal of Chemical Theory and Computation*, **2016**, 12, 1000-10 | 6.4 | 19 |
| 84 | K+ Block Is the Mechanism of Functional Asymmetry in Bacterial Na(v) Channels. *PLoS Computational Biology*, **2016**, 12, e1004482 | 5 | 9 |
| 83 | In silico prediction of drug therapy in catecholaminergic polymorphic ventricular tachycardia. *Journal of Physiology*, **2016**, 594, 567-93 | 3.9 | 28 |
| 82 | BROMOCEA Code: An Improved Grand Canonical Monte Carlo/Brownian Dynamics Algorithm Including Explicit Atoms. *Journal of Chemical Theory and Computation*, **2016**, 12, 2401-17 | 6.4 | 10 |
| 81 | What controls open-pore and residual currents in the first sensing zone of alpha-hemolysin nanopore? Combined experimental and theoretical study. *Nanoscale*, **2016**, 8, 11571-9 | 7.7 | 9 |
| 80 | Current state of theoretical and experimental studies of the voltage-dependent anion channel (VDAC). *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1778-90 | 3.8 | 49 |
| 79 | Improving the LIE Method for Binding Free Energy Calculations of Protein-Ligand Complexes. *Journal of Chemical Information and Modeling*, **2015**, 55, 1867-77 | 6.1 | 23 |
| 78 | BROMOC suite: Monte Carlo/Brownian dynamics suite for studies of ion permeation and DNA transport in biological and artificial pores with effective potentials. *Journal of Computational Chemistry*, **2015**, 36, 264-71 | 3.5 | 8 |
| 77 | NS1643 interacts around L529 of hERG to alter voltage sensor movement on the path to activation. *Biophysical Journal*, **2015**, 108, 1400-1413 | 2.9 | 23 |
| 76 | Elucidating factors important for monovalent cation selectivity in enzymes: E. coli □galactosidase as a model. *Physical Chemistry Chemical Physics*, **2015**, 17, 10899-909 | 3.6 | 27 |
| 75 | Kinetic model for NS1643 drug activation of WT and L529I variants of Kv11.1 (hERG1) potassium channel. *Biophysical Journal*, **2015**, 108, 1414-1424 | 2.9 | 18 |
| 74 | Quantum effects in cation interactions with first and second coordination shell ligands in metalloproteins. *Journal of Chemical Theory and Computation*, **2015**, 11, 4992-5001 | 6.4 | 36 |
| 73 | Mechanism of the Association between Na+ Binding and Conformations at the Intracellular Gate in Neurotransmitter:Sodium Symporters. *Journal of Biological Chemistry*, **2015**, 290, 13992-4003 | 5.4 | 41 |
| 72 | In response to Melgari et al. "hERG potassium channel inhibition by ivabradine requires channel gating". *Journal of Molecular and Cellular Cardiology*, **2015**, 87, 192-3 | 5.8 | |
| 71 | Molecular Simulations of Solved Co-crystallized X-Ray Structures Identify Action Mechanisms of PDE□Inhibitors. *Biophysical Journal*, **2015**, 109, 1163-8 | 2.9 | 13 |
| 70 | Mapping the gating and permeation pathways in the voltage-gated proton channel Hv1. *Journal of Molecular Biology*, **2015**, 427, 131-45 | 6.5 | 22 |

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|---|---|---|---|
| 69 | QM/MM calculations with deMon2k. *Molecules*, **2015**, 20, 4780-812 | 4.8 | 14 |
| 68 | Ivabradine prolongs phase 3 of cardiac repolarization and blocks the hERG1 (KCNH2) current over a concentration-range overlapping with that required to block HCN4. *Journal of Molecular and Cellular Cardiology*, **2015**, 85, 71-8 | 5.8 | 46 |
| 67 | Representation of Ion-Protein Interactions Using the Drude Polarizable Force-Field. *Journal of Physical Chemistry B*, **2015**, 119, 9401-16 | 3.4 | 80 |
| 66 | Magic angle spinning nuclear magnetic resonance characterization of voltage-dependent anion channel gating in two-dimensional lipid crystalline bilayers. *Biochemistry*, **2015**, 54, 994-1005 | 3.2 | 31 |
| 65 | Sodium channel selectivity and conduction: prokaryotes have devised their own molecular strategy. *Journal of General Physiology*, **2014**, 143, 157-71 | 3.4 | 46 |
| 64 | Designing of multi-targeted molecules using combination of molecular screening and in silico drug cardiotoxicity prediction approaches. *Journal of Molecular Graphics and Modelling*, **2014**, 50, 16-34 | 2.8 | 3 |
| 63 | A human ether-□go-go-related (hERG) ion channel atomistic model generated by long supercomputer molecular dynamics simulations and its use in predicting drug cardiotoxicity. *Toxicology Letters*, **2014**, 230, 382-92 | 4.4 | 37 |
| 62 | Microsecond simulations of DNA and ion transport in nanopores with novel ion-ion and ion-nucleotides effective potentials. *Journal of Computational Chemistry*, **2014**, 35, 711-21 | 3.5 | 15 |
| 61 | Molecular strategies to achieve selective conductance in NaK channel variants. *Journal of Physical Chemistry B*, **2014**, 118, 2041-9 | 3.4 | 9 |
| 60 | Rehabilitating drug-induced long-QT promoters: in-silico design of hERG-neutral cisapride analogues with retained pharmacological activity. *BMC Pharmacology & Toxicology*, **2014**, 15, 14 | 2.6 | 14 |
| 59 | Effect of confinement on DNA, solvent and counterion dynamics in a model biological nanopore. *Nanoscale*, **2014**, 6, 9006-16 | 7.7 | 17 |
| 58 | Acidification asymmetrically affects voltage-dependent anion channel implicating the involvement of salt bridges. *Journal of Biological Chemistry*, **2014**, 289, 23670-82 | 5.4 | 36 |
| 57 | Structure driven design of novel human ether-a-go-go-related-gene channel (hERG1) activators. *PLoS ONE*, **2014**, 9, e105553 | 3.7 | 14 |
| 56 | Hydrophobic plug functions as a gate in voltage-gated proton channels. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, E273-82 | 11.5 | 59 |
| 55 | 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). *Physical Chemistry Chemical Physics*, **2013**, 15, 2397-404 | 3.6 | 8 |
| 54 | ATP transport through VDAC and the VDAC-tubulin complex probed by equilibrium and nonequilibrium MD simulations. *Biochemistry*, **2013**, 52, 9246-56 | 3.2 | 45 |
| 53 | Relative Free Energies for Hydration of Monovalent Ions from QM and QM/MM Simulations. *Journal of Chemical Theory and Computation*, **2013**, 9, 4165-75 | 6.4 | 45 |
| 52 | The molecular mechanism of ion-dependent gating in secondary transporters. *PLoS Computational Biology*, **2013**, 9, e1003296 | 5 | 44 |

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|---|---|---|---|
| 51 | Cholesterol sensitivity of KIR2.1 depends on functional inter-links between the N and C termini. *Channels*, **2013**, 7, 303-12 | 3 | 18 |
| 50 | Identification of novel cholesterol-binding regions in Kir2 channels. *Journal of Biological Chemistry*, **2013**, 288, 31154-64 | 5.4 | 77 |
| 49 | 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. *Journal of Pharmacology and Experimental Therapeutics*, **2012**, 342, 441-52 | 4.7 | 25 |
| 48 | Atomistic models of ion and solute transport by the sodium-dependent secondary active transporters. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 337-47 | 3.8 | 20 |
| 47 | Modeling of open, closed, and open-inactivated states of the hERG1 channel: structural mechanisms of the state-dependent drug binding. *Journal of Chemical Information and Modeling*, **2012**, 52, 2760-74 | 6.1 | 60 |
| 46 | Ion-controlled conformational dynamics in the outward-open transition from an occluded state of LeuT. *Biophysical Journal*, **2012**, 103, 878-88 | 2.9 | 77 |
| 45 | BROMOC-D: Brownian Dynamics/Monte-Carlo Program Suite to Study Ion and DNA Permeation in Nanopores. *Journal of Chemical Theory and Computation*, **2012**, 8, 2540-2551 | 6.4 | 24 |
| 44 | The Role of Atomic Polarization in the Thermodynamics of Chloroform Partitioning to Lipid Bilayers. *Journal of Chemical Theory and Computation*, **2012**, 8, 618-28 | 6.4 | 42 |
| 43 | 4-(4-(dimethylamino)phenyl)-1-methylpyridinium (APP+) is a fluorescent substrate for the human serotonin transporter. *Journal of Biological Chemistry*, **2012**, 287, 8852-63 | 5.4 | 38 |
| 42 | 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)). *Journal of Biological Chemistry*, **2012**, 287, 40266-78 | 5.4 | 24 |
| 41 | The structural pathway for water permeation through sodium-glucose cotransporters. *Biophysical Journal*, **2011**, 101, 1887-95 | 2.9 | 35 |
| 40 | Combined receptor and ligand-based approach to the universal pharmacophore model development for studies of drug blockade to the hERG1 pore domain. *Journal of Chemical Information and Modeling*, **2011**, 51, 463-74 | 6.1 | 77 |
| 39 | The role of local hydration and hydrogen-bonding dynamics in ion and solute release from ion-coupled secondary transporters. *Biochemistry*, **2011**, 50, 1848-56 | 3.2 | 47 |
| 38 | A conserved asparagine residue in transmembrane segment 1 (TM1) of serotonin transporter dictates chloride-coupled neurotransmitter transport. *Journal of Biological Chemistry*, **2011**, 286, 30823-30836 | 5.4 | 31 |
| 37 | Atomistic models for free energy evaluation of drug binding to membrane proteins. *Current Medicinal Chemistry*, **2011**, 18, 2601-11 | 4.3 | 16 |
| 36 | Mechanism of K+/Na+ selectivity in potassium channels from the perspective of the non-selective bacterial channel NaK. *Channels*, **2011**, 5, 198-200 | 3 | 5 |
| 35 | Importance of hydration and dynamics on the selectivity of the KcsA and NaK channels. *Journal of General Physiology*, **2011**, 138, 651-651 | 3.4 | 2 |
| 34 | Ion selectivity in channels and transporters. *Journal of General Physiology*, **2011**, 137, 415-26 | 3.4 | 127 |

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| 33 | Evidence for a third sodium-binding site in glutamate transporters suggests an ion/substrate coupling model. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 13912-7 | 11.5 | 69 |
| 32 | Insights into the molecular mechanism of hERG1 channel activation and blockade by drugs. *Current Medicinal Chemistry*, **2010**, 17, 3514-32 | 4.3 | 45 |
| 31 | Two mechanisms of ion selectivity in protein binding sites. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 20329-34 | 11.5 | 69 |
| 30 | The RCK2 domain uses a coordination site present in Kir channels to confer sodium sensitivity to Slo2.2 channels. *Journal of Neuroscience*, **2010**, 30, 7554-62 | 6.6 | 42 |
| 29 | Evaluations of the Absolute and Relative Free Energies for Antidepressant Binding to the Amino Acid Membrane Transporter LeuT with Free Energy Simulations. *Journal of Chemical Theory and Computation*, **2010**, 6, 1900-14 | 6.4 | 23 |
| 28 | Halothane solvation in water and organic solvents from molecular simulations with new polarizable potential function. *Journal of Physical Chemistry B*, **2010**, 114, 6401-8 | 3.4 | 4 |
| 27 | Model of ionic currents through microtubule nanopores and the lumen. *Physical Review E*, **2010**, 81, 051912 | 2.4 | 26 |
| 26 | A Guide to QM/MM Methodology and Applications. *Advances in Quantum Chemistry*, **2010**, 59, 353-400 | 1.4 | 24 |
| 25 | The QM-MM interface for CHARMM-deMon. *Journal of Computational Chemistry*, **2010**, 31, 1015-23 | 3.5 | 19 |
| 24 | Na(+), K (+) and Tl(+) hydration from QM/MM computations and MD simulations with a polarizable force field. *Interdisciplinary Sciences, Computational Life Sciences*, **2010**, 2, 12-20 | 3.5 | 4 |
| 23 | Structural refinement of the hERG1 pore and voltage-sensing domains with ROSETTA-membrane and molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2922-34 | 4.2 | 44 |
| 22 | Pendular proteins in gases and new avenues for characterization of macromolecules by ion mobility spectrometry. *Proceedings of the National Academy of Sciences of the United States of America*, **2009** , 106, 6495-500 | 11.5 | 34 |
| 21 | Polarizable model of chloroform based on classical Drude oscillators. *Chemical Physics Letters*, **2009** , 468, 270-274 | 2.5 | 19 |
| 20 | Hydration number, topological control, and ion selectivity. *Journal of Physical Chemistry B*, **2009**, 113, 8725-30 | 3.4 | 34 |
| 19 | 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. *Biophysical Journal*, **2009**, 96, 3600-10 | 2.9 | 35 |
| 18 | Molecular mechanism of ion-ion and ion-substrate coupling in the Na+-dependent leucine transporter LeuT. *Biophysical Journal*, **2008**, 95, 4613-21 | 2.9 | 52 |
| 17 | Control of ion selectivity in LeuT: two Na+ binding sites with two different mechanisms. *Journal of Molecular Biology*, **2008**, 377, 804-18 | 6.5 | 160 |
| 16 | A three-dimensional model of a group II intron RNA and its interaction with the intron-encoded reverse transcriptase. *Molecular Cell*, **2008**, 30, 472-85 | 17.6 | 60 |

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|---|---|---|---|
| 15 | Molecular mechanism of substrate specificity in the bacterial neutral amino acid transporter LeuT. *Proteins: Structure, Function and Bioinformatics*, **2008**, 73, 851-63 | 4.2 | 32 |
| 14 | Importance of hydration and dynamics on the selectivity of the KcsA and NaK channels. *Journal of General Physiology*, **2007**, 129, 135-43 | 3.4 | 159 |
| 13 | 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, 1587-97 | 6.4 | 123 |
| 12 | Ion selectivity in potassium channels. *Biophysical Chemistry*, **2006**, 124, 279-91 | 3.5 | 144 |
| 11 | Molecular dynamics study of hydration in ethanol-water mixtures using a polarizable force field. *Journal of Physical Chemistry B*, **2005**, 109, 6705-13 | 3.4 | 246 |
| 10 | Control of ion selectivity in potassium channels by electrostatic and dynamic properties of carbonyl ligands. *Nature*, **2004**, 431, 830-4 | 50.4 | 453 |
| 9 | Ion permeation through the alpha-hemolysin channel: theoretical studies based on Brownian dynamics and Poisson-Nernst-Plank electrodiffusion theory. *Biophysical Journal*, **2004**, 87, 2299-309 | 2.9 | 163 |
| 8 | Long-Range Effects of Mutating R248 to Q/W in the p53 Core Domain. *Journal of Physical Chemistry B*, **2002**, 106, 13047-13057 | 3.4 | 7 |
| 7 | Structure of methanol-methanol associates in dilute methanol-water mixtures from molecular dynamics simulation. *Journal of Molecular Liquids*, **2001**, 91, 157-165 | 6 | 26 |
| 6 | The study of hydrophobic hydration in supercritical water-methanol mixtures. *Journal of Molecular Graphics and Modelling*, **2001**, 19, 412-6 | 2.8 | 17 |
| 5 | Free energy decomposition of protein-protein interactions. *Biophysical Journal*, **2001**, 81, 737-50 | 2.9 | 97 |
| 4 | Electron Diffraction and Quantum Chemical Study of the Molecular Structure of para-Methylbenzenesulfonyl Fluoride and para-Methylbenzenesulfonyl Bromide. *Journal of Structural Chemistry*, **2000**, 41, 939-947 | 0.9 | 12 |
| 3 | 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. *Journal of Theoretical and Computational Chemistry*,2042001 | 1.8 | 1 |
| 2 | C subunit of the ATP synthase is an amyloidogenic channel-forming peptide: possible implications in mitochondrial pathogenesis | | 1 |
| 1 | Atomistic modeling towards predictive cardiotoxicity | | 2 |