Maria G Kurnikova

List of Publications by Year
in descending order

66	2,111	257450	243625
papers	citations	24 h-index	44 g-index

68	68	68	1874
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Lattice Relaxation Algorithm for Three-Dimensional Poisson-Nernst-Planck Theory with Application to Ion Transport through the Gramicidin A Channel. Biophysical Journal, 1999, 76, 642-656.	0.5	254
2	Three-Dimensional Poisson-Nernst-Planck Theory Studies: Influence of Membrane Electrostatics on Gramicidin A Channel Conductance. Biophysical Journal, 2000, 79, 80-93.	0.5	163
3	The Role of the Dielectric Barrier in Narrow Biological Channels: A Novel Composite Approach to Modeling Single-Channel Currents. Biophysical Journal, 2003, 84, 3646-3661.	0.5	111
4	Poissonâ€“Nernstâ€“Planck Theory Approach to the Calculation of Current Through Biological Ion Channels. IEEE Transactions on Nanobioscience, 2005, 4, 81-93.	3.3	105
5	Structural Bases of Noncompetitive Inhibition of AMPA-Subtype Ionotropic Glutamate Receptors by Antiepileptic Drugs. Neuron, 2016, 91, 1305-1315.	8.1	103
6	Comparison of Dynamic Lattice Monte Carlo Simulations and the Dielectric Self-Energy Poissonâ^'Nernstâ^'Planck Continuum Theory for Model Ion Channels. Journal of Physical Chemistry B, 2004, 108, 2006-2015.	2.6	93
7	A Dynamic Lattice Monte Carlo Model of Ion Transport in Inhomogeneous Dielectric Environments:Â Method and Implementation. Journal of Physical Chemistry B, 2000, 104, 12324-12338.	2.6	86
8	Diffusion constant of K+ inside Gramicidin A: A comparative study of four computational methods. Biophysical Chemistry, 2006, 124, 268-278.	2.8	74
9	Rotational Relaxation in Polar Solvents. Molecular Dynamics Study of Soluteâ^'Solvent Interaction. Journal of the American Chemical Society, 1998, 120, 6121-6130.	13.7	69
10	Protein flexibility using constraints from molecular dynamics simulations. Physical Biology, 2005, 2, S137-S147.	1.8	58
11	A molecular dynamics study of dielectric friction. Journal of Chemical Physics, 1996, 105, 628-638.	3.0	50
12	Structural Fluctuations, Spin, Reorganization Energy, and Tunneling Energy Control of Intramolecular Electron Transfer:Â The Surprising Case of Electron Transfer in a d8â^'d8Bimetallic System. Journal of the American Chemical Society, 1997, 119, 5690-5700.	13.7	44
13	Epoxidation Catalyzed by the Nonheme Iron(II)- and 2-Oxoglutarate-Dependent Oxygenase, AsqJ: Mechanistic Elucidation of Oxygen Atom Transfer by a Ferryl Intermediate. Journal of the American Chemical Society, 2020, 142, 6268-6284.	13.7	44
14	Stability and rigidity/flexibilityâ€”Two sides of the same coin?. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 854-866.	2.3	43
15	Insights into the Desaturation of Cyclopeptin and its C3 Epimer Catalyzed by a nonâ€Heme Iron Enzyme: Structural Characterization and Mechanism Elucidation. Angewandte Chemie - International Edition, 2018, 57, 1831-1835.	13.8	43
16	pH-Triggered Conformational Switching of the Diphtheria Toxin T-Domain: The Roles of N-Terminal Histidines. Journal of Molecular Biology, 2013, 425, 2752-2764.	4.2	42
17	Structural Basis for NHERF1 PDZ Domain Binding. Biochemistry, 2012, 51, 3110-3120.	2.5	33
18	Role of the Ion Channel Extracellular Collar in AMPA Receptor Gating. Scientific Reports, 2017, 7, 1050.	3.3	33

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19	Ion Permeation Mechanism in Epithelial Calcium Channel TRVP6. Scientific Reports, 2018, 8, 5715.	3.3	30
20	Opening of glutamate receptor channel to subconductance levels. Nature, 2022, 605, 172-178.	27.8	30
21	Structure and function of the calciumâ€selective TRP channel TRPV6. Journal of Physiology, 2021, 599, 2673-2697.	2.9	29
22	Soft Wall Ion Channel in Continuum Representation with Application to Modeling Ion Currents in Î±-Hemolysin. Journal of Physical Chemistry B, 2010, 114, 15180-15190.	2.6	28
23	On the Binding Determinants of the Glutamate Agonist with the Glutamate Receptor Ligand Binding Domain. Biochemistry, 2005, 44, 11508-11517.	2.5	27
24	An Online Approach for Mining Collective Behaviors from Molecular Dynamics Simulations. Journal of Computational Biology, 2010, 17, 309-324.	1.6	27
25	Spontaneous field potentials in the glomeruli of the olfactory bulb: The leading role of juxtaglomerular cells. Neuroscience, 2006, 142, 203-221.	2.3	26
26	Homology modeling and molecular dynamics simulations of the glycine receptor ligand binding domain. Proteins: Structure, Function and Bioinformatics, 2007, 67, 950-960.	2.6	26
27	Rotational diffusion of organic solutes: the role of dielectric friction in polar solvents and electrolyte solutions. Journal of Molecular Liquids, 1998, 77, 37-60.	4.9	25
28	Exploring Protein Stability by Comparative Molecular Dynamics Simulations of Homologous Hyperthermophilic, Mesophilic, and Psychrophilic Proteins. Journal of Chemical Information and Modeling, 2016, 56, 2129-2139.	5.4	25
29	Accurate theoretical prediction of vibrational frequencies in an inhomogeneous dynamic environment: A case study of a glutamate molecule in water solution and in a protein-bound form. Journal of Chemical Physics, 2004, 121, 1516-1524.	3.0	23
30	All atom NMDA receptor transmembrane domain model development and simulations in lipid bilayers and water. PLoS ONE, 2017, 12, e0177686.	2.5	23
31	Energetics of the Cleft Closing Transition and the Role of Electrostatic Interactions in Conformational Rearrangements of the Glutamate Receptor Ligand Binding Domain. Biochemistry, 2008, 47, 11077-11085.	2.5	21
32	Role of Acidic Residues in Helices TH8â€“TH9 in Membrane Interactions of the Diphtheria Toxin T Domain. Toxins, 2015, 7, 1303-1323.	3.4	20
33	Computational Modeling of Poly(alkylthiophene) Conductive Polymer Insertion into Phospholipid Bilayers. Langmuir, 2007, 23, 10672-10681.	3.5	16
34	Interplay between structural rigidity and electrostatic interactions in the ligand binding domain of GluR2. Proteins: Structure, Function and Bioinformatics, 2008, 73, 656-671.	2.6	16
35	Targeting Electrostatic Interactions in Accelerated Molecular Dynamics with Application to Protein Partial Unfolding. Journal of Chemical Theory and Computation, 2015, 11, 2550-2559.	5.3	15
36	Rotational Relaxation of Ionic Molecules in Electrolyte Solutions. Anisotropy Relaxation and Molecular Dynamics Study. Journal of the American Chemical Society, 1998, 120, 7944-7951.	13.7	14

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37	Energetics and Dynamics of a Cyclic Oligosaccharide Molecule in a Confined Protein Pore Environment. A Molecular Dynamics Study. Journal of Physical Chemistry B, 2003, 107, 7189-7201.	2.6	14
38	FLEXIBILITY AND MOBILITY IN MESOPHILIC AND THERMOPHILIC HOMOLOGOUS PROTEINS FROM MOLECULAR DYNAMICS AND FOLDUNFOLD METHOD. Journal of Bioinformatics and Computational Biology, 2010, 08, 377-394.	0.8	14
39	Structural basis of AMPA receptor inhibition by transâ€4â€butylcyclohexane carboxylic acid. British Journal of Pharmacology, 2022, 179, 3628-3644.	5.4	14
40	Accurate determination of solvation free energies of neutral organic compounds from first principles. Nature Communications, 2022, 13, 414.	12.8	14
41	Modeling Electronic Polarizability Changes in the Course of a Magnesium Ion Water Ligand Exchange Process. Journal of Physical Chemistry B, 2015, 119, 10275-10286.	2.6	13
42	AMPA Receptor Noncompetitive Inhibitors Occupy a Promiscuous Binding Site. ACS Chemical Neuroscience, 2019, 10, 4511-4521.	3.5	13
43	Development and initial testing of an empirical forcefield for simulation of poly(alkylthiophenes). Journal of Molecular Graphics and Modelling, 2008, 27, 34-44.	2.4	12
44	The Hydrophobic Effect Contributes to the Closed State of a Simplified Ion Channel through a Conserved Hydrophobic Patch at the Pore-Helix Crossing. Frontiers in Pharmacology, 2015, 6, 284.	3.5	12
45	Inhibition of NMDA receptors through a membrane-to-channel path. Nature Communications, 2022, 13, .	12.8	11
46	Overexpression and Functional Characterization of the Extracellular Domain of the Human Î±1 Glycine Receptor. Biochemistry, 2008, 47, 9803-9810.	2.5	10
47	Membrane Association of the Diphtheria Toxin Translocation Domain Studied by Coarse-Grained Simulations and Experiment. Journal of Membrane Biology, 2015, 248, 529-543.	2.1	10
48	Design, synthesis, and in vitro and in vivo characterization of new memantine analogs for Alzheimer's disease. European Journal of Medicinal Chemistry, 2022, 236, 114354.	5.5	10
49	Structural mechanism of TRPM7 channel regulation by intracellular magnesium. Cellular and Molecular Life Sciences, 2022, 79, 225.	5.4	10
50	Protein stability and dynamics influenced by ligands in extremophilic complexes â€“ a molecular dynamics investigation. Molecular BioSystems, 2017, 13, 1874-1887.	2.9	9
51	Harnessing the Substrate Promiscuity of Dioxygenase AsqJ and Developing Efficient Chemoenzymatic Synthesis for Quinolones. ACS Catalysis, 2021, 11, 7186-7192.	11.2	8
52	Crosslinking Constraints and Computational Models as Complementary Tools in Modeling the Extracellular Domain of the Glycine Receptor. PLoS ONE, 2014, 9, e102571.	2.5	8
53	Microsecond Simulations of the Diphtheria Toxin Translocation Domain in Association with Anionic Lipid Bilayers. Journal of Physical Chemistry B, 2015, 119, 12074-12085.	2.6	7
54	Molecular mechanisms of bio-catalysis of heme extraction from hemoglobin. Redox Biology, 2017, 11, 516-523.	9.0	7

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55	Structure and Energetics of Channel-Forming Proteinâ˜Polysaccharide Complexes Inferred via Computational Statistical Thermodynamics. Journal of Physical Chemistry B, 2006, 110, 25091-25100.	2.6	6
56	An Online Approach for Mining Collective Behaviors from Molecular Dynamics Simulations. Lecture Notes in Computer Science, 2009, , 138-154.	1.3	6
57	Configurational Preference of the Glutamate Receptor Ligand Binding Domain Dimers. Biophysical Journal, 2017, 112, 2291-2300.	0.5	5
58	Characterizing the Energetic States of the GluR2 Ligand Binding Domain Core-Dimer. Biophysical Journal, 2011, 100, L5-L7.	0.5	4
59	Membrane Position Dependency of the pKa and Conductivity of the Protein Ion Channel. Journal of Membrane Biology, 2018, 251, 393-404.	2.1	4
60	A Hierarchical Approach to Predict Conformation-Dependent Histidine Protonation States in Stable and Flexible Proteins. Journal of Physical Chemistry B, 2019, 123, 5024-5034.	2.6	4
61	Poissonâ€“Nernstâ€“Planck Theory of Ion Permeation Through Biological Channels. , 2007, , 449-484.		4
62	Modeling of peptides connecting the ligandâ€binding and transmembrane domains in the GluR2 glutamate receptor. Proteins: Structure, Function and Bioinformatics, 2009, 76, 271-280.	2.6	3
63	Insights into the Desaturation of Cyclopeptin and its C3 Epimer Catalyzed by a nonâ€Heme Iron Enzyme: Structural Characterization and Mechanism Elucidation. Angewandte Chemie, 2018, 130, 1849-1853.	2.0	3
64	A molecular dynamics study of photothermal compression of colloidal crystals. Journal of Chemical Physics, 1997, 106, 1585-1592.	3.0	2
65	Computational prediction of ion permeation characteristics in the glycine receptor modified by photo-sensitive compounds. Journal of Computer-Aided Molecular Design, 2008, 22, 563-570.	2.9	2
66	Baseline Comparisons of Complementary Sampling Methods for Assembly Driven by Short-Ranged Pair Potentials toward Fast and Flexible Hybridization. Journal of Chemical Theory and Computation, 2021, 17, 1967-1987.	5.3	2