Jerry M Parks

List of Publications by Year
in descending order

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109 papers	4,466 citations	109321 35 h-index	123424 61 g-index
119 all docs	119 docs citations	119 times ranked	6396 citing authors

#	Article	IF	Citations
1	Hit Expansion of a Noncovalent SARS-CoV-2 Main Protease Inhibitor. ACS Pharmacology and Translational Science, 2022, 5, 255-265.	4.9	17
2	AF2Complex predicts direct physical interactions in multimeric proteins with deep learning. Nature Communications, 2022, 13, 1744.	12.8	128
3	OpenMDlr: parallel, open-source tools for general protein structure modeling and refinement from pairwise distances. Bioinformatics, 2022, 38, 3297-3298.	4.1	0
4	Property space mapping of Pseudomonas aeruginosa permeability to small molecules. Scientific Reports, 2022, 12, 8220.	3.3	9
5	Core cysteine residues in the Plasminogen-Apple-Nematode (PAN) domain are critical for HGF/c-MET signaling. Communications Biology, 2022, 5, .	4.4	5
6	Î²-Barrel proteins tether the outer membrane in many Gram-negative bacteria. Nature Microbiology, 2021, 6, 19-26.	13.3	46
7	Machine learningâ€based prediction of enzyme substrate scope: Application to bacterial nitrilases. Proteins: Structure, Function and Bioinformatics, 2021, 89, 336-347.	2.6	30
8	Antitumor T-cell Immunity Contributes to Pancreatic Cancer Immune Resistance. Cancer Immunology Research, 2021, 9, 386-400.	3.4	9
9	Multidrug Efflux Pumps and the Two-Faced Janus of Substrates and Inhibitors. Accounts of Chemical Research, 2021, 54, 930-939.	15.6	25
10	Probing the oligomeric re-assembling of bacterial fimbriae in vitro: a small-angle X-ray scattering and analytical ultracentrifugation study. European Biophysics Journal, 2021, 50, 597-611.	2.2	3
11	Hotspot Coevolution Is a Key Identifier of Near-Native Protein Complexes. Journal of Physical Chemistry B, 2021, 125, 6058-6067.	2.6	1
12	Editorial: Advances in computational molecular biophysics. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129888.	2.4	0
13	Mechanistic Investigation of Dimethylmercury Formation Mediated by a Sulfide Mineral Surface. Journal of Physical Chemistry A, 2021, 125, 5397-5405.	2.5	3
14	Machine Learning Reveals the Critical Interactions for SARS-CoV-2 Spike Protein Binding to ACE2. Journal of Physical Chemistry Letters, 2021, 12, 5494-5502.	4.6	44
15	Pretreatment with Sodium Methyl Mercaptide Increases Carbohydrate Yield during Kraft Pulping. ACS Sustainable Chemistry and Engineering, 2021, 9, 11571-11580.	6.7	3
16	Mechanistic Duality of Bacterial Efflux Substrates and Inhibitors: Example of Simple Substituted Cinnamoyl and Naphthyl Amides. ACS Infectious Diseases, 2021, 7, 2650-2665.	3.8	16
17	Lpp positions peptidoglycan at the AcrA-TolC interface in the AcrAB-TolC multidrug efflux pump. Biophysical Journal, 2021, 120, 3973-3982.	0.5	13
18	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. Chemical Science, 2021, 12, 1513-1527.	7.4	47

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19	The AQUAâ€MER databases and aqueous speciation server: A web resource for multiscale modeling of mercury speciation. Journal of Computational Chemistry, 2020, 41, 147-155.	3.3	3
20	A Minimal Membrane Metal Transport System: Dynamics and Energetics of mer Proteins. Journal of Computational Chemistry, 2020, 41, 528-537.	3.3	5
21	Molecular Dynamics Simulation of the Structures, Dynamics, and Aggregation of Dissolved Organic Matter. Environmental Science & Technology, 2020, 54, 13527-13537.	10.0	36
22	Combining Three-Dimensional Modeling with Artificial Intelligence to Increase Specificity and Precision in Peptideâ€“MHC Binding Predictions. Journal of Immunology, 2020, 205, 1962-1977.	0.8	7
23	Insight into the Catalytic Mechanism of GH11 Xylanase: Computational Analysis of Substrate Distortion Based on a Neutron Structure. Journal of the American Chemical Society, 2020, 142, 17966-17980.	13.7	13
24	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. Journal of Chemical Information and Modeling, 2020, 60, 5832-5852.	5.4	134
25	How to Discover Antiviral Drugs Quickly. New England Journal of Medicine, 2020, 382, 2261-2264.	27.0	76
26	Structure determination of the HgcAB complex using metagenome sequence data: insights into microbial mercury methylation. Communications Biology, 2020, 3, 320.	4.4	30
27	Discovery of multidrug efflux pump inhibitors with a novel chemical scaffold. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129546.	2.4	33
28	Co(salen)-Catalyzed Oxidation of Lignin Models to Form Benzoquinones and Benzaldehydes: A Computational and Experimental Study. ACS Sustainable Chemistry and Engineering, 2020, 8, 7225-7234.	6.7	18
29	Studying the surfaces of bacteria using neutron scattering: finding new openings for antibiotics. Biochemical Society Transactions, 2020, 48, 2139-2149.	3.4	5
30	Helix N-Cap Residues Drive the Acid Unfolding That Is Essential in the Action of the Toxin Colicin A. Biochemistry, 2019, 58, 4882-4892.	2.5	1
31	Horizontal transfer of a pathway for coumarate catabolism unexpectedly inhibits purine nucleotide biosynthesis. Molecular Microbiology, 2019, 112, 1784-1797.	2.5	5
32	Ligand-Dependent Sodium Ion Dynamics within the A_{2A} Adenosine Receptor: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2019, 123, 7947-7954.	2.6	4
33	Conformational Dynamics of AcrA Govern Multidrug Efflux Pump Assembly. ACS Infectious Diseases, 2019, 5, 1926-1935.	3.8	21
34	A probabilistic perspective on thermodynamic parameter uncertainties: Understanding aqueous speciation of mercury. Geochimica Et Cosmochimica Acta, 2019, 263, 108-121.	3.9	4
35	Identification of Binding Sites for Efflux Pump Inhibitors of the AcrAB-TolC Component AcrA. Biophysical Journal, 2019, 116, 648-658.	0.5	27
36	Environmental Mercury Chemistry â€“ In Silico. Accounts of Chemical Research, 2019, 52, 379-388.	15.6	40

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37	Engineered mosaic protein polymers; a simple route to multifunctional biomaterials. Journal of Biological Engineering, 2019, 13, 54.	4.7	7
38	Mercury Uptake by Desulfovibrio desulfuricans ND132: Passive or Active?. Environmental Science & Technology, 2019, 53, 6264-6272.	10.0	33
39	Kinetics of Enzymatic Mercury Methylation at Nanomolar Concentrations Catalyzed by HgcAB. Applied and Environmental Microbiology, 2019, 85, .	3.1	20
40	Induction of the immunoprotective coat of Yersinia pestis at body temperature is mediated by the Caf1R transcription factor. BMC Microbiology, 2019, 19, 68.	3.3	7
41	Exceptional response and multisystem autoimmune-like toxicities associated with the same T cell clone in a patient with uveal melanoma treated with immune checkpoint inhibitors. , 2019, 7, 61.		40
42	Targeted isolation and cultivation of uncultivated bacteria by reverse genomics. Nature Biotechnology, 2019, 37, 1314-1321.	17.5	231
43	Substrate Binding Induces Conformational Changes in a Class A Î²-lactamase That Prime It for Catalysis. ACS Catalysis, 2018, 8, 2428-2437.	11.2	27
44	Quantum Chemical Calculation of pK_as of Environmentally Relevant Functional Groups: Carboxylic Acids, Amines, and Thiols in Aqueous Solution. Journal of Physical Chemistry A, 2018, 122, 4366-4374.	2.5	62
45	Emerging investigator series: methylmercury speciation and dimethylmercury production in sulfidic solutions. Environmental Sciences: Processes and Impacts, 2018, 20, 584-594.	3.5	17
46	Mycolyltransferase from Mycobacterium tuberculosis in covalent complex with tetrahydrolipstatin provides insights into antigen 85 catalysis. Journal of Biological Chemistry, 2018, 293, 3651-3662.	3.4	16
47	Development of CHARMM-Compatible Force-Field Parameters for Cobalamin and Related Cofactors from Quantum Mechanical Calculations. Journal of Chemical Theory and Computation, 2018, 14, 784-798.	5.3	20
48	Impact of hydration and temperature history on the structure and dynamics of lignin. Green Chemistry, 2018, 20, 1602-1611.	9.0	30
49	Distribution of mechanical stress in the Escherichia coli cell envelope. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 2566-2575.	2.6	66
50	Quantum Chemical Approach for Calculating Stability Constants of Mercury Complexes. ACS Earth and Space Chemistry, 2018, 2, 1168-1178.	2.7	14
51	Molecular Properties That Define the Activities of Antibiotics in Escherichia coli and Pseudomonas aeruginosa. ACS Infectious Diseases, 2018, 4, 1223-1234.	3.8	54
52	Modular Protein Engineering Approach to the Functionalization of Gold Nanoparticles for Use in Clinical Diagnostics. ACS Applied Nano Materials, 2018, 1, 3590-3599.	5.0	9
53	Tuneable hydrogels of Caf1 protein fibers. Materials Science and Engineering C, 2018, 93, 88-95.	7.3	9
54	Liquid crystalline bacterial outer membranes are critical for antibiotic susceptibility. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7587-E7594.	7.1	67

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55	Quantitative Proteomic Analysis of Biological Processes and Responses of the Bacterium Desulfovibrio desulfuricans ND132 upon Deletion of Its Mercury Methylation Genes. Proteomics, 2018, 18, e1700479.	2.2	22
56	Hyperconjugation Promotes Catalysis in a Pyridoxal 5â€²-Phosphate-Dependent Enzyme. ACS Catalysis, 2018, 8, 6733-6737.	11.2	15
57	Direct evidence that an extended hydrogen-bonding network influences activation of pyridoxal 5â€²-phosphate in aspartate aminotransferase. Journal of Biological Chemistry, 2017, 292, 5970-5980.	3.4	38
58	Toward the rational design of macrolide antibiotics to combat resistance. Chemical Biology and Drug Design, 2017, 90, 641-652.	3.2	10
59	Exploring Covalent Allosteric Inhibition of Antigen 85C from Mycobacterium tuberculosis by Ebselen Derivatives. ACS Infectious Diseases, 2017, 3, 378-387.	3.8	26
60	Identification of Mercury and Dissolved Organic Matter Complexes Using Ultrahigh Resolution Mass Spectrometry. Environmental Science and Technology Letters, 2017, 4, 59-65.	8.7	43
61	Active-Site Protonation States in an Acyl-Enzyme Intermediate of a Class A Î²-Lactamase with a Monobactam Substrate. Antimicrobial Agents and Chemotherapy, 2017, 61, .	3.2	26
62	Direct visualization of critical hydrogen atoms in a pyridoxal 5â€²-phosphate enzyme. Nature Communications, 2017, 8, 955.	12.8	55
63	Modeling of the Passive Permeation of Mercury and Methylmercury Complexes Through a Bacterial Cytoplasmic Membrane. Environmental Science & Technology, 2017, 51, 10595-10604.	10.0	15
64	The Two-State Prehensile Tail of the Antibacterial Toxin Colicin N. Biophysical Journal, 2017, 113, 1673-1684.	0.5	18
65	Identification and Structureâ€“Activity Relationships of Novel Compounds that Potentiate the Activities of Antibiotics in Escherichia coli. Journal of Medicinal Chemistry, 2017, 60, 6205-6219.	6.4	45
66	Reviving Antibiotics: Efflux Pump Inhibitors That Interact with AcrA, a Membrane Fusion Protein of the AcrAB-TolC Multidrug Efflux Pump. ACS Infectious Diseases, 2017, 3, 89-98.	3.8	88
67	Longâ€Range ElectrostaticsâEInduced Twoâ€Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. Angewandte Chemie, 2016, 128, 5008-5011.	2.0	6
68	Longâ€Range ElectrostaticsâEInduced Twoâ€Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. Angewandte Chemie - International Edition, 2016, 55, 4924-4927.	13.8	42
69	Gram-negative trimeric porins have specific LPS binding sites that are essential for porin biogenesis. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E5034-43.	7.1	103
70	Modeling Mercury in Proteins. Methods in Enzymology, 2016, 578, 103-122.	1.0	9
71	Toward Quantitatively Accurate Calculation of the Redox-Associated Acidâ€“Base and Ligand Binding Equilibria of Aquacobalamin. Journal of Physical Chemistry B, 2016, 120, 7307-7318.	2.6	3
72	Site-Directed Mutagenesis of HgcA and HgcB Reveals Amino Acid Residues Important for Mercury Methylation. Applied and Environmental Microbiology, 2015, 81, 3205-3217.	3.1	73

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73	HackaMol: An Object-Oriented Modern Perl Library for Molecular Hacking on Multiple Scales. Journal of Chemical Information and Modeling, 2015, 55, 721-726.	5.4	6
74	Direct determination of protonation states and visualization of hydrogen bonding in a glycoside hydrolase with neutron crystallography. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12384-12389.	7.1	35
75	Antibacterial toxin colicin N and phage protein G3p compete with TolB for a binding site on TolA. Microbiology (United Kingdom), 2015, 161, 503-515.	1.8	14
76	Protein Kinase A Catalytic Subunit Primed for Action: Time-Lapse Crystallography of Michaelis Complex Formation. Structure, 2015, 23, 2331-2340.	3.3	22
77	High coverage fluid-phase floating lipid bilayers supported by Ï‰-thiolipid self-assembled monolayers. Journal of the Royal Society Interface, 2014, 11, 20140447.	3.4	22
78	X-ray Structure of a Hg²⁺ Complex of Mercuric Reductase (MerA) and Quantum Mechanical/Molecular Mechanical Study of Hg²⁺ Transfer between the C-Terminal and Buried Catalytic Site Cysteine Pairs. Biochemistry, 2014, 53, 7211-7222.	2.5	46
79	Chemical Factors that Control Lignin Polymerization. Journal of Physical Chemistry B, 2014, 118, 164-170.	2.6	46
80	Structure and Dynamics of a Compact State of a Multidomain Protein, the Mercuric Ion Reductase. Biophysical Journal, 2014, 107, 393-400.	0.5	19
81	Unexpected Effects of Gene Deletion on Interactions of Mercury with the Methylation-Deficient Mutant Î”hgcAB. Environmental Science and Technology Letters, 2014, 1, 271-276.	8.7	22
82	L-Arabinose Binding, Isomerization, and Epimerization by D-Xylose Isomerase: X-Ray/Neutron Crystallographic and Molecular Simulation Study. Structure, 2014, 22, 1287-1300.	3.3	22
83	Mercury Methylation by HgcA: Theory Supports Carbanion Transfer to Hg(II). Inorganic Chemistry, 2014, 53, 772-777.	4.0	34
84	Hydrolysis of DFP and the Nerve Agent (S)-Sarin by DFPase Proceeds along Two Different Reaction Pathways: Implications for Engineering Bioscavengers. Journal of Physical Chemistry B, 2014, 118, 4479-4489.	2.6	42
85	Why Mercury Prefers Soft Ligands. Journal of Physical Chemistry Letters, 2013, 4, 2317-2322.	4.6	54
86	Comparative Informatics Analysis to Evaluate Site-Specific Protein Oxidation in Multidimensional LCâ€“MS/MS Data. Journal of Proteome Research, 2013, 12, 3307-3316.	3.7	13
87	Cluster-Continuum Calculations of Hydration Free Energies of Anions and Group 12 Divalent Cations. Journal of Chemical Theory and Computation, 2013, 9, 555-569.	5.3	44
88	The Genetic Basis for Bacterial Mercury Methylation. Science, 2013, 339, 1332-1335.	12.6	778
89	Structural Characterization of a Model Gram-Negative Bacterial Surface Using Lipopolysaccharides from Rough Strains of Escherichia coli. Biomacromolecules, 2013, 14, 2014-2022.	5.4	76
90	Pseudobond parameters for QM/MM studies involving nucleosides, nucleotides, and their analogs. Journal of Chemical Physics, 2013, 138, 045102.	3.0	5

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91	Benchmark Interaction Energies for Biologically Relevant Noncovalent Complexes Containing Divalent Sulfur. Journal of Physical Chemistry A, 2012, 116, 1086-1092.	2.5	48
92	Radical Coupling Reactions in Lignin Synthesis: A Density Functional Theory Study. Journal of Physical Chemistry B, 2012, 116, 4760-4768.	2.6	101
93	Down-regulation of the caffeic acid O-methyltransferase gene in switchgrass reveals a novel monolignol analog. Biotechnology for Biofuels, 2012, 5, 71.	6.2	96
94	Molecular Simulation in the Energy Biosciences. RSC Biomolecular Sciences, 2012, , 87-114.	0.4	0
95	Molecular simulation as a tool for studying lignin. Environmental Progress and Sustainable Energy, 2012, 31, 47-54.	2.3	56
96	Mercury Detoxification by Bacteria: Simulations of Transcription Activation and Mercuryï£¿Carbon Bond Cleavage. , 2011, , 311-324.		0
97	Structural Characterization of Intramolecular Hg2+ Transfer between Flexibly Linked Domains of Mercuric Ion Reductase. Journal of Molecular Biology, 2011, 413, 639-656.	4.2	24
98	Mutant alcohol dehydrogenase leads to improved ethanol tolerance in Clostridium thermocellum. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 13752-13757.	7.1	159
99	Structure and Conformational Dynamics of the Metalloregulator MerR upon Binding of Hg(II). Journal of Molecular Biology, 2010, 398, 555-568.	4.2	32
100	Mechanism of Cdc25B Phosphatase with the Small Molecule Substrate p-Nitrophenyl Phosphate from QM/MM-MFEP Calculations. Journal of Physical Chemistry B, 2009, 113, 5217-5224.	2.6	25
101	Mechanism of Hgâ^'C Protonolysis in the Organomercurial Lyase MerB. Journal of the American Chemical Society, 2009, 131, 13278-13285.	13.7	70
102	Hepatitis C Virus NS5B Polymerase:â€‰ QM/MM Calculations Show the Important Role of the Internal Energy in Ligand Binding. Journal of Physical Chemistry B, 2008, 112, 3168-3176.	2.6	14
103	A pseudobond parametrization for improved electrostatics in quantum mechanical/molecular mechanical simulations of enzymes. Journal of Chemical Physics, 2008, 129, 154106.	3.0	31
104	Quantum mechanics/molecular mechanics minimum free-energy path for accurate reaction energetics in solution and enzymes: Sequential sampling and optimization on the potential of mean force surface. Journal of Chemical Physics, 2008, 128, 034105.	3.0	110
105	Experimental Validation of the Docking Orientation of Cdc25 with Its Cdk2â^'CycA Protein Substrateâ€. Biochemistry, 2005, 44, 16563-16573.	2.5	43
106	Quantum Chemical Characterization of the Reactions of Guanine with the Phenylnitrenium Ion. Journal of Organic Chemistry, 2001, 66, 8997-9004.	3.2	24
107	Discovery of critical Tol A-binding residues in the bactericidal toxin colicin N: a biophysical approach. Molecular Microbiology, 1998, 28, 1335-1343.	2.5	58
108	Displacement of OmpF loop 3 is not required for the membrane translocation of colicins N and A in vivo. FEBS Letters, 1998, 432, 117-122.	2.8	22

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109	Macromolecular organisation of recombinant Yersinia pestis F1 antigen and the effect of structure on immunogenicity. FEMS Immunology and Medical Microbiology, 1998, 21, 213-221.	2.7	1