

# Jerry M Parks

## List of Publications by Year in descending order

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109  
papers

4,466  
citations

109137

35  
h-index

123241

61  
g-index

119  
all docs

119  
docs citations

119  
times ranked

6396  
citing authors

#	ARTICLE	IF	CITATIONS
1	The Genetic Basis for Bacterial Mercury Methylation. <i>Science</i> , 2013, 339, 1332-1335.	6.0	778
2	Targeted isolation and cultivation of uncultivated bacteria by reverse genomics. <i>Nature Biotechnology</i> , 2019, 37, 1314-1321.	9.4	231
3	Mutant alcohol dehydrogenase leads to improved ethanol tolerance in <i>Clostridium thermocellum</i> . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 13752-13757.	3.3	159
4	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5832-5852.	2.5	134
5	AF2Complex predicts direct physical interactions in multimeric proteins with deep learning. <i>Nature Communications</i> , 2022, 13, 1744.	5.8	128
6	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. <i>Journal of Chemical Physics</i> , 2008, 128, 034105.	1.2	110
7	Gram-negative trimeric porins have specific LPS binding sites that are essential for porin biogenesis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E5034-43.	3.3	103
8	Radical Coupling Reactions in Lignin Synthesis: A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 4760-4768.	1.2	101
9	Down-regulation of the caffeic acid O-methyltransferase gene in switchgrass reveals a novel monolignol analog. <i>Biotechnology for Biofuels</i> , 2012, 5, 71.	6.2	96
10	Reviving Antibiotics: Efflux Pump Inhibitors That Interact with AcrA, a Membrane Fusion Protein of the AcrAB-TolC Multidrug Efflux Pump. <i>ACS Infectious Diseases</i> , 2017, 3, 89-98.	1.8	88
11	Structural Characterization of a Model Gram-Negative Bacterial Surface Using Lipopolysaccharides from Rough Strains of <i>Escherichia coli</i> . <i>Biomacromolecules</i> , 2013, 14, 2014-2022.	2.6	76
12	How to Discover Antiviral Drugs Quickly. <i>New England Journal of Medicine</i> , 2020, 382, 2261-2264.	13.9	76
13	Site-Directed Mutagenesis of HgcA and HgcB Reveals Amino Acid Residues Important for Mercury Methylation. <i>Applied and Environmental Microbiology</i> , 2015, 81, 3205-3217.	1.4	73
14	Mechanism of Hg <sup>2+</sup> C Protonolysis in the Organomercurial Lyase MerB. <i>Journal of the American Chemical Society</i> , 2009, 131, 13278-13285.	6.6	70
15	Liquid crystalline bacterial outer membranes are critical for antibiotic susceptibility. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E7587-E7594.	3.3	67
16	Distribution of mechanical stress in the <i>Escherichia coli</i> cell envelope. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 2566-2575.	1.4	66
17	Quantum Chemical Calculation of pK <sub>a</sub> s of Environmentally Relevant Functional Groups: Carboxylic Acids, Amines, and Thiols in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4366-4374.	1.1	62
18	Discovery of critical Tol A-binding residues in the bactericidal toxin colicin N: a biophysical approach. <i>Molecular Microbiology</i> , 1998, 28, 1335-1343.	1.2	58

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19	Molecular simulation as a tool for studying lignin. <i>Environmental Progress and Sustainable Energy</i> , 2012, 31, 47-54.	1.3	56
20	Direct visualization of critical hydrogen atoms in a pyridoxal 5â€²-phosphate enzyme. <i>Nature Communications</i> , 2017, 8, 955.	5.8	55
21	Why Mercury Prefers Soft Ligands. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2317-2322.	2.1	54
22	Molecular Properties That Define the Activities of Antibiotics in <i>Escherichia coli</i> and <i>Pseudomonas aeruginosa</i> . <i>ACS Infectious Diseases</i> , 2018, 4, 1223-1234.	1.8	54
23	Benchmark Interaction Energies for Biologically Relevant Noncovalent Complexes Containing Divalent Sulfur. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1086-1092.	1.1	48
24	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. <i>Chemical Science</i> , 2021, 12, 1513-1527.	3.7	47
25	X-ray Structure of a Hg <sup>2+</sup> Complex of Mercuric Reductase (MerA) and Quantum Mechanical/Molecular Mechanical Study of Hg <sup>2+</sup> Transfer between the C-Terminal and Buried Catalytic Site Cysteine Pairs. <i>Biochemistry</i> , 2014, 53, 7211-7222.	1.2	46
26	Chemical Factors that Control Lignin Polymerization. <i>Journal of Physical Chemistry B</i> , 2014, 118, 164-170.	1.2	46
27	Î²-Barrel proteins tether the outer membrane in many Gram-negative bacteria. <i>Nature Microbiology</i> , 2021, 6, 19-26.	5.9	46
28	Identification and Structure-Activity Relationships of Novel Compounds that Potentiate the Activities of Antibiotics in <i>Escherichia coli</i> . <i>Journal of Medicinal Chemistry</i> , 2017, 60, 6205-6219.	2.9	45
29	Cluster-Continuum Calculations of Hydration Free Energies of Anions and Group 12 Divalent Cations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 555-569.	2.3	44
30	Machine Learning Reveals the Critical Interactions for SARS-CoV-2 Spike Protein Binding to ACE2. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5494-5502.	2.1	44
31	Experimental Validation of the Docking Orientation of Cdc25 with Its Cdk2-CycA Protein Substrate. <i>Biochemistry</i> , 2005, 44, 16563-16573.	1.2	43
32	Identification of Mercury and Dissolved Organic Matter Complexes Using Ultrahigh Resolution Mass Spectrometry. <i>Environmental Science and Technology Letters</i> , 2017, 4, 59-65.	3.9	43
33	Hydrolysis of DFP and the Nerve Agent ( <i>S</i> )-Sarin by DFPase Proceeds along Two Different Reaction Pathways: Implications for Engineering Bioscavengers. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4479-4489.	1.2	42
34	Long-Range Electrostatics-Induced Two-Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 4924-4927.	7.2	42
35	Environmental Mercury Chemistry â€œ In Silico. <i>Accounts of Chemical Research</i> , 2019, 52, 379-388.	7.6	40
36	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

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37	Direct evidence that an extended hydrogen-bonding network influences activation of pyridoxal 5â€²-phosphate in aspartate aminotransferase. <i>Journal of Biological Chemistry</i> , 2017, 292, 5970-5980.	1.6	38
38	Molecular Dynamics Simulation of the Structures, Dynamics, and Aggregation of Dissolved Organic Matter. <i>Environmental Science &amp; Technology</i> , 2020, 54, 13527-13537.	4.6	36
39	Direct determination of protonation states and visualization of hydrogen bonding in a glycoside hydrolase with neutron crystallography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 12384-12389.	3.3	35
40	Mercury Methylation by HgcA: Theory Supports Carbanion Transfer to Hg(II). <i>Inorganic Chemistry</i> , 2014, 53, 772-777.	1.9	34
41	Mercury Uptake by <i>Desulfovibrio desulfuricans</i> ND132: Passive or Active?. <i>Environmental Science &amp; Technology</i> , 2019, 53, 6264-6272.	4.6	33
42	Discovery of multidrug efflux pump inhibitors with a novel chemical scaffold. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2020, 1864, 129546.	1.1	33
43	Structure and Conformational Dynamics of the Metalloregulator MerR upon Binding of Hg(II). <i>Journal of Molecular Biology</i> , 2010, 398, 555-568.	2.0	32
44	A pseudobond parametrization for improved electrostatics in quantum mechanical/molecular mechanical simulations of enzymes. <i>Journal of Chemical Physics</i> , 2008, 129, 154106.	1.2	31
45	Impact of hydration and temperature history on the structure and dynamics of lignin. <i>Green Chemistry</i> , 2018, 20, 1602-1611.	4.6	30
46	Structure determination of the HgcAB complex using metagenome sequence data: insights into microbial mercury methylation. <i>Communications Biology</i> , 2020, 3, 320.	2.0	30
47	Machine learning-based prediction of enzyme substrate scope: Application to bacterial nitrilases. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 336-347.	1.5	30
48	Substrate Binding Induces Conformational Changes in a Class A $\beta$ -lactamase That Prime It for Catalysis. <i>ACS Catalysis</i> , 2018, 8, 2428-2437.	5.5	27
49	Identification of Binding Sites for Efflux Pump Inhibitors of the AcrAB-TolC Component AcrA. <i>Biophysical Journal</i> , 2019, 116, 648-658.	0.2	27
50	Exploring Covalent Allosteric Inhibition of Antigen 85C from <i>Mycobacterium tuberculosis</i> by Ebselen Derivatives. <i>ACS Infectious Diseases</i> , 2017, 3, 378-387.	1.8	26
51	Active-Site Protonation States in an Acyl-Enzyme Intermediate of a Class A $\beta$ -Lactamase with a Monobactam Substrate. <i>Antimicrobial Agents and Chemotherapy</i> , 2017, 61, .	1.4	26
52	Mechanism of Cdc25B Phosphatase with the Small Molecule Substrate <i>p</i> -Nitrophenyl Phosphate from QM/MM-MFEP Calculations. <i>Journal of Physical Chemistry B</i> , 2009, 113, 5217-5224.	1.2	25
53	Multidrug Efflux Pumps and the Two-Faced Janus of Substrates and Inhibitors. <i>Accounts of Chemical Research</i> , 2021, 54, 930-939.	7.6	25
54	Quantum Chemical Characterization of the Reactions of Guanine with the Phenylnitrenium Ion. <i>Journal of Organic Chemistry</i> , 2001, 66, 8997-9004.	1.7	24

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55	Structural Characterization of Intramolecular Hg <sup>2+</sup> Transfer between Flexibly Linked Domains of Mercuric Ion Reductase. <i>Journal of Molecular Biology</i> , 2011, 413, 639-656.	2.0	24
56	Displacement of OmpF loop 3 is not required for the membrane translocation of colicins N and A in vivo. <i>FEBS Letters</i> , 1998, 432, 117-122.	1.3	22
57	High coverage fluid-phase floating lipid bilayers supported by 1% thiolipid self-assembled monolayers. <i>Journal of the Royal Society Interface</i> , 2014, 11, 20140447.	1.5	22
58	Unexpected Effects of Gene Deletion on Interactions of Mercury with the Methylation-Deficient Mutant HgcAB. <i>Environmental Science and Technology Letters</i> , 2014, 1, 271-276.	3.9	22
59	L-Arabinose Binding, Isomerization, and Epimerization by D-Xylose Isomerase: X-Ray/Neutron Crystallographic and Molecular Simulation Study. <i>Structure</i> , 2014, 22, 1287-1300.	1.6	22
60	Protein Kinase A Catalytic Subunit Primed for Action: Time-Lapse Crystallography of Michaelis Complex Formation. <i>Structure</i> , 2015, 23, 2331-2340.	1.6	22
61	Quantitative Proteomic Analysis of Biological Processes and Responses of the Bacterium <i>Desulfovibrio desulfuricans</i> ND132 upon Deletion of Its Mercury Methylation Genes. <i>Proteomics</i> , 2018, 18, e1700479.	1.3	22
62	Conformational Dynamics of AcrA Govern Multidrug Efflux Pump Assembly. <i>ACS Infectious Diseases</i> , 2019, 5, 1926-1935.	1.8	21
63	Development of CHARMM-Compatible Force-Field Parameters for Cobalamin and Related Cofactors from Quantum Mechanical Calculations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 784-798.	2.3	20
64	Kinetics of Enzymatic Mercury Methylation at Nanomolar Concentrations Catalyzed by HgcAB. <i>Applied and Environmental Microbiology</i> , 2019, 85, .	1.4	20
65	Structure and Dynamics of a Compact State of a Multidomain Protein, the Mercuric Ion Reductase. <i>Biophysical Journal</i> , 2014, 107, 393-400.	0.2	19
66	The Two-State Prehensile Tail of the Antibacterial Toxin Colicin N. <i>Biophysical Journal</i> , 2017, 113, 1673-1684.	0.2	18
67	Co(salen)-Catalyzed Oxidation of Lignin Models to Form Benzoquinones and Benzaldehydes: A Computational and Experimental Study. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 7225-7234.	3.2	18
68	Emerging investigator series: methylmercury speciation and dimethylmercury production in sulfidic solutions. <i>Environmental Sciences: Processes and Impacts</i> , 2018, 20, 584-594.	1.7	17
69	Hit Expansion of a Noncovalent SARS-CoV-2 Main Protease Inhibitor. <i>ACS Pharmacology and Translational Science</i> , 2022, 5, 255-265.	2.5	17
70	Mycyltransferase from <i>Mycobacterium tuberculosis</i> in covalent complex with tetrahydrolipstatin provides insights into antigen 85 catalysis. <i>Journal of Biological Chemistry</i> , 2018, 293, 3651-3662.	1.6	16
71	Mechanistic Duality of Bacterial Efflux Substrates and Inhibitors: Example of Simple Substituted Cinnamoyl and Naphthyl Amides. <i>ACS Infectious Diseases</i> , 2021, 7, 2650-2665.	1.8	16
72	Modeling of the Passive Permeation of Mercury and Methylmercury Complexes Through a Bacterial Cytoplasmic Membrane. <i>Environmental Science &amp; Technology</i> , 2017, 51, 10595-10604.	4.6	15

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73	Hyperconjugation Promotes Catalysis in a Pyridoxal 5â€²-Phosphate-Dependent Enzyme. <i>ACS Catalysis</i> , 2018, 8, 6733-6737.	5.5	15
74	Hepatitis C Virus NS5B Polymerase:â€‰ QM/MM Calculations Show the Important Role of the Internal Energy in Ligand Binding. <i>Journal of Physical Chemistry B</i> , 2008, 112, 3168-3176.	1.2	14
75	Antibacterial toxin colicin N and phage protein G3p compete with TolB for a binding site on TolA. <i>Microbiology (United Kingdom)</i> , 2015, 161, 503-515.	0.7	14
76	Quantum Chemical Approach for Calculating Stability Constants of Mercury Complexes. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 1168-1178.	1.2	14
77	Comparative Informatics Analysis to Evaluate Site-Specific Protein Oxidation in Multidimensional LCâ€‰MS/MS Data. <i>Journal of Proteome Research</i> , 2013, 12, 3307-3316.	1.8	13
78	Insight into the Catalytic Mechanism of GH11 Xylanase: Computational Analysis of Substrate Distortion Based on a Neutron Structure. <i>Journal of the American Chemical Society</i> , 2020, 142, 17966-17980.	6.6	13
79	Lpp positions peptidoglycan at the AcrA-TolC interface in the AcrAB-TolC multidrug efflux pump. <i>Biophysical Journal</i> , 2021, 120, 3973-3982.	0.2	13
80	Toward the rational design of macrolide antibiotics to combat resistance. <i>Chemical Biology and Drug Design</i> , 2017, 90, 641-652.	1.5	10
81	Modeling Mercury in Proteins. <i>Methods in Enzymology</i> , 2016, 578, 103-122.	0.4	9
82	Modular Protein Engineering Approach to the Functionalization of Gold Nanoparticles for Use in Clinical Diagnostics. <i>ACS Applied Nano Materials</i> , 2018, 1, 3590-3599.	2.4	9
83	Tuneable hydrogels of Caf1 protein fibers. <i>Materials Science and Engineering C</i> , 2018, 93, 88-95.	3.8	9
84	Antitumor T-cell Immunity Contributes to Pancreatic Cancer Immune Resistance. <i>Cancer Immunology Research</i> , 2021, 9, 386-400.	1.6	9
85	Property space mapping of <i>Pseudomonas aeruginosa</i> permeability to small molecules. <i>Scientific Reports</i> , 2022, 12, 8220.	1.6	9
86	Engineered mosaic protein polymers; a simple route to multifunctional biomaterials. <i>Journal of Biological Engineering</i> , 2019, 13, 54.	2.0	7
87	Induction of the immunoprotective coat of <i>Yersinia pestis</i> at body temperature is mediated by the Caf1R transcription factor. <i>BMC Microbiology</i> , 2019, 19, 68.	1.3	7
88	Combining Three-Dimensional Modeling with Artificial Intelligence to Increase Specificity and Precision in Peptideâ€‰MHC Binding Predictions. <i>Journal of Immunology</i> , 2020, 205, 1962-1977.	0.4	7
89	HackaMol: An Object-Oriented Modern Perl Library for Molecular Hacking on Multiple Scales. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 721-726.	2.5	6
90	Longâ€‰Range Electrostaticsâ€‰Induced Twoâ€‰Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. <i>Angewandte Chemie</i> , 2016, 128, 5008-5011.	1.6	6

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91	Pseudobond parameters for QM/MM studies involving nucleosides, nucleotides, and their analogs. <i>Journal of Chemical Physics</i> , 2013, 138, 045102.	1.2	5
92	Horizontal transfer of a pathway for coumarate catabolism unexpectedly inhibits purine nucleotide biosynthesis. <i>Molecular Microbiology</i> , 2019, 112, 1784-1797.	1.2	5
93	A Minimal Membrane Metal Transport System: Dynamics and Energetics of <i>mer</i> Proteins. <i>Journal of Computational Chemistry</i> , 2020, 41, 528-537.	1.5	5
94	Studying the surfaces of bacteria using neutron scattering: finding new openings for antibiotics. <i>Biochemical Society Transactions</i> , 2020, 48, 2139-2149.	1.6	5
95	Core cysteine residues in the Plasminogen-Apoptin-Nematode (PAN) domain are critical for HGF/c-MET signaling. <i>Communications Biology</i> , 2022, 5, .	2.0	5
96	Ligand-Dependent Sodium Ion Dynamics within the A <sub>2A</sub> Adenosine Receptor: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7947-7954.	1.2	4
97	A probabilistic perspective on thermodynamic parameter uncertainties: Understanding aqueous speciation of mercury. <i>Geochimica Et Cosmochimica Acta</i> , 2019, 263, 108-121.	1.6	4
98	Toward Quantitatively Accurate Calculation of the Redox-Associated Acid-Base and Ligand Binding Equilibria of Aquacobalamin. <i>Journal of Physical Chemistry B</i> , 2016, 120, 7307-7318.	1.2	3
99	The AQUAMER databases and aqueous speciation server: A web resource for multiscale modeling of mercury speciation. <i>Journal of Computational Chemistry</i> , 2020, 41, 147-155.	1.5	3
100	Probing the oligomeric re-assembling of bacterial fimbriae in vitro: a small-angle X-ray scattering and analytical ultracentrifugation study. <i>European Biophysics Journal</i> , 2021, 50, 597-611.	1.2	3
101	Mechanistic Investigation of Dimethylmercury Formation Mediated by a Sulfide Mineral Surface. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5397-5405.	1.1	3
102	Pretreatment with Sodium Methyl Mercaptide Increases Carbohydrate Yield during Kraft Pulping. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 11571-11580.	3.2	3
103	Helix N-Cap Residues Drive the Acid Unfolding That Is Essential in the Action of the Toxin Colicin A. <i>Biochemistry</i> , 2019, 58, 4882-4892.	1.2	1
104	Hotspot Coevolution Is a Key Identifier of Near-Native Protein Complexes. <i>Journal of Physical Chemistry B</i> , 2021, 125, 6058-6067.	1.2	1
105	Macromolecular organisation of recombinant <i>Yersinia pestis</i> F1 antigen and the effect of structure on immunogenicity. , 0, .		1
106	Mercury Detoxification by Bacteria: Simulations of Transcription Activation and Mercury-Carbon Bond Cleavage. , 2011, , 311-324.		0
107	Molecular Simulation in the Energy Biosciences. <i>RSC Biomolecular Sciences</i> , 2012, , 87-114.	0.4	0
108	Editorial: Advances in computational molecular biophysics. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2021, 1865, 129888.	1.1	0

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109	OpenMDr: parallel, open-source tools for general protein structure modeling and refinement from pairwise distances. <i>Bioinformatics</i> , 2022, 38, 3297-3298.	1.8	0