

Marcelo A Marti

List of Publications by Year in descending order

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169
papers

6,121
citations

53794

45
h-index

106344

65
g-index

178
all docs

178
docs citations

178
times ranked

6830
citing authors

#	ARTICLE	IF	CITATIONS
1	H ₂ S and NO cooperatively regulate vascular tone by activating a neuroendocrine HNO ⁺ TRPA1 ⁺ CGRP signalling pathway. <i>Nature Communications</i> , 2014, 5, 4381.	12.8	324
2	The Catalytic Mechanism of Peptidylglycine β -Hydroxylating Monooxygenase Investigated by Computer Simulation. <i>Journal of the American Chemical Society</i> , 2006, 128, 12817-12828.	13.7	137
3	A DFT-Based QM-MM Approach Designed for the Treatment of Large Molecular Systems: Application to Chorismate Mutase. <i>Journal of Physical Chemistry B</i> , 2003, 107, 13728-13736.	2.6	116
4	Aromatic ⁺ Aromatic Interactions in Proteins: Beyond the Dimer. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 1623-1633.	5.4	115
5	Evidence for a ferryl intermediate in a heme-based dioxygenase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 17371-17376.	7.1	113
6	Multiple-Steering QM ⁺ MM Calculation of the Free Energy Profile in Chorismate Mutase. <i>Journal of the American Chemical Society</i> , 2005, 127, 6940-6941.	13.7	112
7	Theoretical Study of the Truncated Hemoglobin HbN: Exploring the Molecular Basis of the NO Detoxification Mechanism. <i>Journal of the American Chemical Society</i> , 2005, 127, 4433-4444.	13.7	111
8	pH-Dependent Conformational Changes in Proteins and Their Effect on Experimental pK _a s: The Case of Nitrophorin 4. <i>PLoS Computational Biology</i> , 2012, 8, e1002761.	3.2	110
9	Discrimination of Nitroxyl and Nitric Oxide by Water-Soluble Mn(III) Porphyrins. <i>Journal of the American Chemical Society</i> , 2005, 127, 4680-4684.	13.7	109
10	Ligand-induced dynamical regulation of NO conversion in Mycobacterium tuberculosis truncated hemoglobin-N. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 64, 457-464.	2.6	95
11	Heme Protein Oxygen Affinity Regulation Exerted by Proximal Effects. <i>Journal of the American Chemical Society</i> , 2006, 128, 12455-12461.	13.7	91
12	Dioxygen affinity in heme proteins investigated by computer simulation. <i>Journal of Inorganic Biochemistry</i> , 2006, 100, 761-770.	3.5	89
13	Nitroxyl (azanone) trapping by metalloporphyrins. <i>Coordination Chemistry Reviews</i> , 2011, 255, 2764-2784.	18.8	84
14	Fast Nitroxyl Trapping by Ferric Porphyrins. <i>Journal of the American Chemical Society</i> , 2003, 125, 15272-15273.	13.7	82
15	The Structural Biology of Galectin-Ligand Recognition: Current Advances in Modeling Tools, Protein Engineering, and Inhibitor Design. <i>Frontiers in Chemistry</i> , 2019, 7, 823.	3.6	80
16	Free Energy Calculations with Non-Equilibrium Methods: Applications of the Jarzynski Relationship. <i>Theoretical Chemistry Accounts</i> , 2006, 116, 338-346.	1.4	79
17	Nitric Oxide Is Reduced to HNO by Proton-Coupled Nucleophilic Attack by Ascorbate, Tyrosine, and Other Alcohols. A New Route to HNO in Biological Media?. <i>Journal of the American Chemical Society</i> , 2015, 137, 4720-4727.	13.7	79
18	Modeling heme proteins using atomistic simulations. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 5611-5628.	2.8	77

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19	Time-Resolved Electrochemical Quantification of Azanone (HNO) at Low Nanomolar Level. <i>Analytical Chemistry</i> , 2013, 85, 10262-10269.	6.5	73
20	Trapping and Characterization of a Reaction Intermediate in Carbapenem Hydrolysis by <i>B. cereus</i> Metallo- β -lactamase. <i>Journal of the American Chemical Society</i> , 2008, 130, 15852-15863.	13.7	72
21	The NtrY/X two-component system of <i>Brucella</i> spp. acts as a redox sensor and regulates the expression of nitrogen respiration enzymes. <i>Molecular Microbiology</i> , 2012, 85, 39-50.	2.5	72
22	Complete Reaction Mechanism of Indoleamine 2,3-Dioxygenase as Revealed by QM/MM Simulations. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1401-1413.	2.6	68
23	Molecular Dynamics in Mixed Solvents Reveals Protein-Ligand Interactions, Improves Docking, and Allows Accurate Binding Free Energy Predictions. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 846-863.	5.4	68
24	Molecular Basis for the Electric Field Modulation of Cytochrome <i>c</i> Structure and Function. <i>Journal of the American Chemical Society</i> , 2009, 131, 16248-16256.	13.7	66
25	Inhibitory effect of quercetin on matrix metalloproteinase 9 activity Molecular mechanism and structure-activity relationship of the flavonoid-enzyme interaction. <i>European Journal of Pharmacology</i> , 2010, 644, 138-145.	3.5	65
26	Nitric Oxide Interaction with Cytochrome <i>c</i> and Its Relevance to Guanylate Cyclase. Why Does the Iron Histidine Bond Break?. <i>Journal of the American Chemical Society</i> , 2005, 127, 7721-7728.	13.7	64
27	Molecular Basis of Coupled Protein and Electron Transfer Dynamics of Cytochrome <i>c</i> in Biomimetic Complexes. <i>Journal of the American Chemical Society</i> , 2010, 132, 5769-5778.	13.7	64
28	A Surface Effect Allows HNO/NO Discrimination by a Cobalt Porphyrin Bound to Gold. <i>Inorganic Chemistry</i> , 2010, 49, 6955-6966.	4.0	63
29	A Microscopic Study of the Deoxyhemoglobin-Catalyzed Generation of Nitric Oxide from Nitrite Anion. <i>Biochemistry</i> , 2008, 47, 9793-9802.	2.5	62
30	Role of Pre-A Motif in Nitric Oxide Scavenging by Truncated Hemoglobin, HbN, of <i>Mycobacterium tuberculosis</i> . <i>Journal of Biological Chemistry</i> , 2009, 284, 14457-14468.	3.4	59
31	CG2AA: backmapping protein coarse-grained structures. <i>Bioinformatics</i> , 2016, 32, 1235-1237.	4.1	59
32	Reactions of HNO with Metal Porphyrins: Underscoring the Biological Relevance of HNO. <i>Accounts of Chemical Research</i> , 2014, 47, 2907-2916.	15.6	56
33	Whole Genome Sequencing Reveals a De Novo SHANK3 Mutation in Familial Autism Spectrum Disorder. <i>PLoS ONE</i> , 2015, 10, e0116358.	2.5	55
34	Exploring the molecular basis of heme coordination in human neuroglobin. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 71, 695-705.	2.6	54
35	The first step of the dioxygenation reaction carried out by tryptophan dioxygenase and indoleamine 2,3-dioxygenase as revealed by quantum mechanical/molecular mechanical studies. <i>Journal of Biological Inorganic Chemistry</i> , 2010, 15, 811-823.	2.6	53
36	Target-Pathogen: a structural bioinformatic approach to prioritize drug targets in pathogens. <i>Nucleic Acids Research</i> , 2018, 46, D413-D418.	14.5	53

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37	Heme-oxygenase-1 implications in cell morphology and the adhesive behavior of prostate cancer cells. <i>Oncotarget</i> , 2014, 5, 4087-4102.	1.8	53
38	Structural and Molecular Basis of the Peroxynitrite-mediated Nitration and Inactivation of <i>Trypanosoma cruzi</i> Iron-Superoxide Dismutases (Fe-SODs) A and B. <i>Journal of Biological Chemistry</i> , 2014, 289, 12760-12778.	3.4	51
39	An integrative, multi-omics approach towards the prioritization of <i>Klebsiella pneumoniae</i> drug targets. <i>Scientific Reports</i> , 2018, 8, 10755.	3.3	50
40	Dynamical Characterization of the Heme NO Oxygen Binding (HNOX) Domain. Insight into Soluble Guanylate Cyclase Allosteric Transition. <i>Biochemistry</i> , 2008, 47, 9416-9427.	2.5	49
41	Role of Heme Distortion on Oxygen Affinity in Heme Proteins: The Protoglobin Case. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8536-8543.	2.6	49
42	Exploring the molecular basis of human manganese superoxide dismutase inactivation mediated by tyrosine 34 nitration. <i>Archives of Biochemistry and Biophysics</i> , 2011, 507, 304-309.	3.0	48
43	Physiological concentrations of melatonin inhibit the nitridergic pathway in the Syrian hamster retina. <i>Journal of Pineal Research</i> , 2002, 33, 31-36.	7.4	47
44	Structural determinants of ligand migration in <i>Mycobacterium tuberculosis</i> truncated hemoglobin O. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 73, 372-379.	2.6	47
45	Solvent structure improves docking prediction in lectin-carbohydrate complexes. <i>Glycobiology</i> , 2013, 23, 241-258.	2.5	47
46	WATCLUST: a tool for improving the design of drugs based on protein-water interactions. <i>Bioinformatics</i> , 2015, 31, 3697-3699.	4.1	47
47	Systemic Type I IFN Inflammation in Human ISG15 Deficiency Leads to Necrotizing Skin Lesions. <i>Cell Reports</i> , 2020, 31, 107633.	6.4	47
48	Dynamical Regulation of Ligand Migration by a Gate-Opening Molecular Switch in Truncated Hemoglobin-N from <i>Mycobacterium tuberculosis</i> . <i>Journal of the American Chemical Society</i> , 2007, 129, 6782-6788.	13.7	46
49	Insights on Glucocorticoid Receptor Activity Modulation through the Binding of Rigid Steroids. <i>PLoS ONE</i> , 2010, 5, e13279.	2.5	44
50	High pressure reveals structural determinants for globin hexacoordination: Neuroglobin and myoglobin cases. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 75, 885-894.	2.6	43
51	Molecular Basis for the Substrate Stereoselectivity in Tryptophan Dioxygenase. <i>Biochemistry</i> , 2011, 50, 10910-10918.	2.5	42
52	AutoDock Bias: improving binding mode prediction and virtual screening using known protein-ligand interactions. <i>Bioinformatics</i> , 2019, 35, 3836-3838.	4.1	42
53	HNO Is Produced by the Reaction of NO with Thiols. <i>Journal of the American Chemical Society</i> , 2017, 139, 14483-14487.	13.7	41
54	Modulation of the NO trans effect in heme proteins: implications for the activation of soluble guanylate cyclase. <i>Journal of Biological Inorganic Chemistry</i> , 2003, 8, 595-600.	2.6	39

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55	QM Study of Nitrite Reduction by Nitrite Reductase of <i>Pseudomonas aeruginosa</i> . <i>Journal of Physical Chemistry B</i> , 2004, 108, 18073-18080.	2.6	39
56	Comparing and combining implicit ligand sampling with multiple steered molecular dynamics to study ligand migration processes in heme proteins. <i>Journal of Computational Chemistry</i> , 2011, 32, 2219-2231.	3.3	39
57	Protein Topology Determines Cysteine Oxidation Fate: The Case of Sulfenyl Amide Formation among Protein Families. <i>PLoS Computational Biology</i> , 2015, 11, e1004051.	3.2	39
58	Bond or Cage Effect: How Nitrophorins Transport and Release Nitric Oxide. <i>Journal of the American Chemical Society</i> , 2008, 130, 1611-1618.	13.7	38
59	Aromatic clusters in protein-protein and protein-drug complexes. <i>Journal of Cheminformatics</i> , 2020, 12, 30.	6.1	38
60	pH-Dependent Mechanism of Nitric Oxide Release in Nitrophorins 2 and 4. <i>Journal of Physical Chemistry B</i> , 2009, 113, 1192-1201.	2.6	37
61	Small ligand-globin interactions: Reviewing lessons derived from computer simulation. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2013, 1834, 1722-1738.	2.3	37
62	Redox Potential Determines the Reaction Mechanism of HNO Donors with Mn and Fe Porphyrins: Defining the Better Traps. <i>Inorganic Chemistry</i> , 2014, 53, 7351-7360.	4.0	37
63	Mechanism of the Reaction of Human Manganese Superoxide Dismutase with Peroxynitrite: Nitration of Critical Tyrosine 34. <i>Biochemistry</i> , 2016, 55, 3403-3417.	2.5	37
64	Thermal Fluctuations Determine the Electron Transfer Rates of Cytochrome c in Electrostatic and Covalent Complexes. <i>ChemPhysChem</i> , 2010, 11, 1225-1235.	2.1	36
65	Unraveling the molecular basis for ligand binding in truncated hemoglobins: The trHbO <i>Bacillus subtilis</i> case. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 962-970.	2.6	36
66	Discussing Endogenous NO/HNO Interconversion Aided by Phenolic Drugs and Vitamins. <i>Inorganic Chemistry</i> , 2015, 54, 9342-9350.	4.0	36
67	Evolutionary and Functional Relationships in the Truncated Hemoglobin Family. <i>PLoS Computational Biology</i> , 2016, 12, e1004701.	3.2	36
68	HNO trapping and assisted decomposition of nitroxyl donors by ferric hemes. <i>Polyhedron</i> , 2007, 26, 4673-4679.	2.2	35
69	Mechanism of Product Release in NO Detoxification from <i>Mycobacterium tuberculosis</i> Truncated Hemoglobin N. <i>Journal of the American Chemical Society</i> , 2008, 130, 1688-1693.	13.7	35
70	Substrate stereospecificity in tryptophan dioxygenase and indoleamine 2,3-dioxygenase. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 2961-2972.	2.6	35
71	TuberQ: a <i>Mycobacterium tuberculosis</i> protein druggability database. <i>Database: the Journal of Biological Databases and Curation</i> , 2014, 2014, bau035-bau035.	3.0	35
72	Oxygen affinity controlled by dynamical distal conformations: The soybean leghemoglobin and the <i>Paramecium caudatum</i> hemoglobin cases. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 68, 480-487.	2.6	33

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73	Carbohydrate-Binding Proteins: Dissecting Ligand Structures through Solvent Environment Occupancy. <i>Journal of Physical Chemistry B</i> , 2009, 113, 8717-8724.	2.6	33
74	Computer simulation and SERR detection of cytochrome c dynamics at SAM-coated electrodes. <i>Electrochimica Acta</i> , 2009, 54, 4963-4970.	5.2	32
75	Characterization of the Galectin-1 Carbohydrate Recognition Domain in Terms of Solvent Occupancy. <i>Journal of Physical Chemistry B</i> , 2007, 111, 7360-7366.	2.6	31
76	Ligand Migration in <i>Methanosarcina acetivorans</i> Protoglobin: Effects of Ligand Binding and Dimeric Assembly. <i>Journal of Physical Chemistry B</i> , 2011, 115, 13771-13780.	2.6	31
77	Molecular basis of intramolecular electron transfer in proteins during radical-mediated oxidations: Computer simulation studies in model tyrosine-cysteine peptides in solution. <i>Archives of Biochemistry and Biophysics</i> , 2012, 525, 82-91.	3.0	31
78	Protein dynamics and ligand migration interplay as studied by computer simulation. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011, 1814, 1054-1064.	2.3	30
79	Molecular Dynamics Simulations Provide Atomistic Insight into Hydrogen Exchange Mass Spectrometry Experiments. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 658-669.	5.3	30
80	Heme oxygenase-1 in the forefront of a multi-molecular network that governs cell-cell contacts and filopodia-induced zippering in prostate cancer. <i>Cell Death and Disease</i> , 2016, 7, e2570-e2570.	6.3	30
81	An optimized methodology for whole genome sequencing of RNA respiratory viruses from nasopharyngeal aspirates. <i>PLoS ONE</i> , 2018, 13, e0199714.	2.5	30
82	Hydrophobic Effect Drives Oxygen Uptake in Myoglobin via Histidine E7. <i>Journal of Biological Chemistry</i> , 2013, 288, 6754-6762.	3.4	28
83	QM/MM study of the C-C coupling reaction mechanism of CYP121, an essential Cytochrome p450 of <i>Mycobacterium tuberculosis</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 1004-1021.	2.6	28
84	The hemoglobins of the sub-Antarctic fish <i>Cottoperca gobio</i> , a phylogenetically basal species oxygen-binding equilibria, kinetics and molecular dynamics. <i>FEBS Journal</i> , 2009, 276, 2266-2277.	4.7	27
85	Nitric Oxide Reactivity with Globins as Investigated Through Computer Simulation. <i>Methods in Enzymology</i> , 2008, 437, 477-498.	1.0	26
86	Structural Model for p75NTR-TrkA Intracellular Domain Interaction: A Combined FRET and Bioinformatics Study. <i>Journal of Molecular Biology</i> , 2011, 414, 681-698.	4.2	26
87	Role of PheE15 Gate in Ligand Entry and Nitric Oxide Detoxification Function of <i>Mycobacterium tuberculosis</i> Truncated Hemoglobin N. <i>PLoS ONE</i> , 2012, 7, e49291.	2.5	26
88	Underlying Thermodynamics of pH-Dependent Allostery. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12818-12826.	2.6	26
89	Solvents to Fragments to Drugs: MD Applications in Drug Design. <i>Molecules</i> , 2018, 23, 3269.	3.8	25
90	Environment effects on chemical reactivity of heme proteins. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 1505-1514.	2.0	23

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91	An Integrated Computational Analysis of the Structure, Dynamics, and Ligand Binding Interactions of the Human Galectin Network. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 1918-1930.	5.4	23
92	Role of the Distal Hydrogen-Bonding Network in Regulating Oxygen Affinity in the Truncated Hemoglobin III from <i>Campylobacter jejuni</i> . <i>Biochemistry</i> , 2011, 50, 3946-3956.	2.5	23
93	Structural basis for ligand recognition in a mushroom lectin: solvent structure as specificity predictor. <i>Carbohydrate Research</i> , 2011, 346, 939-948.	2.3	23
94	Ligand Migration in the Apolar Tunnel of <i>Cerebratulus lacteus</i> Mini-Hemoglobin. <i>Journal of Biological Chemistry</i> , 2011, 286, 5347-5358.	3.4	23
95	Molecular Mechanism of Myoglobin Autoxidation: Insights from Computer Simulations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1802-1813.	2.6	23
96	Tertiary and quaternary structural basis of oxygen affinity in human hemoglobin as revealed by multiscale simulations. <i>Scientific Reports</i> , 2017, 7, 10926.	3.3	23
97	High-throughput splicing assays identify missense and silent splice-disruptive POU1F1 variants underlying pituitary hormone deficiency. <i>American Journal of Human Genetics</i> , 2021, 108, 1526-1539.	6.2	23
98	Exploring the Molecular Basis of Action of the Passive Antiglucocorticoid 21-Hydroxy-6,19-epoxyprogesterone. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 1352-1360.	6.4	22
99	Two distinct heme distal site states define <i>Cerebratulus lacteus</i> mini-hemoglobin oxygen affinity. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 62, 641-648.	2.6	21
100	The peculiar heme pocket of the 2/2 hemoglobin of cold-adapted <i>Pseudoalteromonas haloplanktis</i> TAC125. <i>Journal of Biological Inorganic Chemistry</i> , 2011, 16, 299-311.	2.6	21
101	Structural Study of a Flexible Active Site Loop in Human Indoleamine 2,3-Dioxygenase and Its Functional Implications. <i>Biochemistry</i> , 2016, 55, 2785-2793.	2.5	21
102	A whole genome bioinformatic approach to determine potential latent phase specific targets in <i>Mycobacterium tuberculosis</i> . <i>Tuberculosis</i> , 2016, 97, 181-192.	1.9	21
103	Cosolvent-Based Protein Pharmacophore for Ligand Enrichment in Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3572-3583.	5.4	21
104	Engineered chimeras reveal the structural basis of hexacoordination in globins: A case study of neuroglobin and myoglobin. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 169-177.	2.4	20
105	Allelic differences in a vacuolar invertase affect <i>Arabidopsis</i> growth at early plant development. <i>Journal of Experimental Botany</i> , 2016, 67, 4091-4103.	4.8	20
106	Germline and somatic mutations in cortical malformations: Molecular defects in Argentinean patients with neuronal migration disorders. <i>PLoS ONE</i> , 2017, 12, e0185103.	2.5	20
107	Molecular Basis for the pH Dependent Structural Transition of Nitrophorin 4. <i>Journal of Physical Chemistry B</i> , 2009, 113, 2135-2142.	2.6	19
108	A protective protein matrix improves the discrimination of nitroxyl from nitric oxide by MnIII protoporphyrinate IX in aerobic media. <i>Journal of Inorganic Biochemistry</i> , 2011, 105, 1044-1049.	3.5	19

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109	CDK2 and PKA Mediated-Sequential Phosphorylation Is Critical for p19INK4d Function in the DNA Damage Response. <i>PLoS ONE</i> , 2012, 7, e35638.	2.5	19
110	Using crystallographic water properties for the analysis and prediction of lectin-carbohydrate complex structures. <i>Glycobiology</i> , 2015, 25, 181-196.	2.5	19
111	Linking the Structure and Thermal Stability of β -Galactoside-Binding Protein Galectin-1 to Ligand Binding and Dimerization Equilibria. <i>Biochemistry</i> , 2010, 49, 7652-7658.	2.5	18
112	Structural Insights into the HWE Histidine Kinase Family: The Brucella Blue Light-Activated Histidine Kinase Domain. <i>Journal of Molecular Biology</i> , 2016, 428, 1165-1179.	4.2	18
113	Genetics and genomic medicine in Argentina. <i>Molecular Genetics & Genomic Medicine</i> , 2018, 6, 481-491.	1.2	17
114	Next generation sequencing panel based on single molecule molecular inversion probes for detecting genetic variants in children with hypopituitarism. <i>Molecular Genetics & Genomic Medicine</i> , 2018, 6, 514-525.	1.2	17
115	Gordon Holmes Syndrome Caused by RNF216 Novel Mutation in 2 Argentinean Siblings. <i>Movement Disorders Clinical Practice</i> , 2019, 6, 259-262.	1.5	17
116	Proximal effects in the modulation of nitric oxide synthase reactivity: a QM-MM study. <i>Journal of Biological Inorganic Chemistry</i> , 2005, 10, 595-604.	2.6	16
117	Hemisuccinate of 21 α -Hydroxy Δ ^{6,19} -Epoxyprogesterone: A Tissue-Specific Modulator of the Glucocorticoid Receptor. <i>ChemMedChem</i> , 2008, 3, 1869-1877.	3.2	16
118	From Genome to Drugs: New Approaches in Antimicrobial Discovery. <i>Frontiers in Pharmacology</i> , 2021, 12, 647060.	3.5	16
119	Probing the Chemotaxis Periplasmic Sensor Domains from <i>Geobacter sulfurreducens</i> by Combined Resonance Raman and Molecular Dynamic Approaches: NO and CO Sensing. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11251-11260.	2.6	15
120	Mechanistic Insight into the Enzymatic Reduction of Truncated Hemoglobin N of <i>Mycobacterium tuberculosis</i> . <i>Journal of Biological Chemistry</i> , 2014, 289, 21573-21583.	3.4	15
121	A quantitative model for oxygen uptake and release in a family of heme proteins. <i>Bioinformatics</i> , 2016, 32, 1805-1813.	4.1	15
122	Kinase Activation by Small Conformational Changes. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 821-832.	5.4	15
123	Clamping, bending, and twisting inter-domain motions in the misfold-recognizing portion of UDP-glucose: Glycoprotein glucosyltransferase. <i>Structure</i> , 2021, 29, 357-370.e9.	3.3	15
124	A Remote Secondary Binding Pocket Promotes Heteromultivalent Targeting of DC-SIGN. <i>Journal of the American Chemical Society</i> , 2021, 143, 18977-18988.	13.7	15
125	Protonation of histidine 55 affects the oxygen access to heme in the alpha chain of the hemoglobin from the Antarctic fish <i>Trematomus bernacchii</i> . <i>IUBMB Life</i> , 2011, 63, 175-182.	3.4	14
126	Improving Efficiency in SMD Simulations Through a Hybrid Differential Relaxation Algorithm. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4609-4617.	5.3	14

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127	Tyrosine oxidation and nitration in transmembrane peptides is connected to lipid peroxidation. <i>Archives of Biochemistry and Biophysics</i> , 2017, 622, 9-25.	3.0	14
128	Rapid Whole-Cell Assay of Antitubercular Drugs Using Second-Generation Fluoromycobacteriophages. <i>Antimicrobial Agents and Chemotherapy</i> , 2016, 60, 3253-3256.	3.2	13
129	Electron transfer dynamics of <i>Rhodothermus marinus</i> caa3 cytochrome c domains on biomimetic films. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18088.	2.8	12
130	Draft Genome Sequence of <i>Bizionia argentinensis</i> , Isolated from Antarctic Surface Water. <i>Journal of Bacteriology</i> , 2011, 193, 6797-6798.	2.2	12
131	Structure and function of crocodilian hemoglobins and allosteric regulation by chloride, ATP, and CO ₂ . <i>American Journal of Physiology - Regulatory Integrative and Comparative Physiology</i> , 2020, 318, R657-R667.	1.8	12
132	p38 ^β Activation Triggers Dynamical Changes in Allosteric Docking Sites. <i>Biochemistry</i> , 2011, 50, 1384-1395.	2.5	11
133	Multiscale approach to the activation and phosphotransfer mechanism of CpxA histidine kinase reveals a tight coupling between conformational and chemical steps. <i>Biochemical and Biophysical Research Communications</i> , 2018, 498, 305-312.	2.1	11
134	Ligand uptake in <i>Mycobacterium tuberculosis</i> truncated hemoglobins is controlled by both internal tunnels and active site water molecules. <i>F1000Research</i> , 2015, 4, 22.	1.6	11
135	Quaternary structure effects on the hexacoordination equilibrium in rice hemoglobin rHb1: Insights from molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013, 81, 863-873.	2.6	10
136	Coarse-Grained Simulations of Heme Proteins: Validation and Study of Large Conformational Transitions. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3390-3397.	5.3	10
137	Single nucleotide polymorphisms may explain the contrasting phenotypes of two variants of a multidrug-resistant <i>Mycobacterium tuberculosis</i> strain. <i>Tuberculosis</i> , 2017, 103, 28-36.	1.9	10
138	VarQ: A Tool for the Structural and Functional Analysis of Human Protein Variants. <i>Frontiers in Genetics</i> , 2018, 9, 620.	2.3	10
139	The key role of water in the dioxygenase function of <i>Escherichia coli</i> flavohemoglobin. <i>Journal of Inorganic Biochemistry</i> , 2013, 119, 75-84.	3.5	9
140	Theoretical Insights into the Reaction and Inhibition Mechanism of Metal-Independent Retaining Glycosyltransferase Responsible for Mycothiol Biosynthesis. <i>Journal of Physical Chemistry B</i> , 2017, 121, 471-478.	2.6	9
141	Biased Docking for Protein-Ligand Pose Prediction. <i>Methods in Molecular Biology</i> , 2021, 2266, 39-72.	0.9	9
142	Thyroid Hormone Interactions with DMPC Bilayers. A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2009, 113, 13357-13364.	2.6	8
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