

# Marcelo A Marti

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/6181792/publications.pdf>

Version: 2024-02-01

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	MotSASi: Functional short linear motifs (SLiMs) prediction based on genomic single nucleotide variants and structural data. <i>Biochimie</i> , 2022, 197, 59-73.	2.6	3
2	Specificity and Reactivity of <i>Mycobacterium tuberculosis</i> Serine/Threonine Kinases PknG and PknB. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1723-1733.	5.4	3
3	Pulmonary Alveolar Proteinosis and Multiple Infectious Diseases in a Child with Autosomal Recessive Complete IRF8 Deficiency. <i>Journal of Clinical Immunology</i> , 2022, 42, 975-985.	3.8	7
4	<i>Mycobacterium tuberculosis</i> DosS binds H <sub>2</sub> S through its Fe <sup>3+</sup> heme iron to regulate the DosR dormancy regulon. <i>Redox Biology</i> , 2022, 52, 102316.	9.0	8
5	Structural modeling of a novel membrane-bound globin-coupled sensor in <i>Geobacter sulfurreducens</i> . <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 1874-1888.	4.1	1
6	Oculocutaneous albinism type 1B associated with a functionally significant tyrosinase gene polymorphism detected with Whole Exome Sequencing. <i>Ophthalmic Genetics</i> , 2021, 42, 291-295.	1.2	3
7	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
8	From Genome to Drugs: New Approaches in Antimicrobial Discovery. <i>Frontiers in Pharmacology</i> , 2021, 12, 647060.	3.5	16
9	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
10	Biased Docking for Protein-Ligand Pose Prediction. <i>Methods in Molecular Biology</i> , 2021, 2266, 39-72.	0.9	9
11	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
12	Conformational and Reaction Dynamic Coupling in Histidine Kinases: Insights from Hybrid QM/MM Simulations. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 833-842.	5.4	8
13	Kinase Activation by Small Conformational Changes. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 821-832.	5.4	15
14	Systemic Type I IFN Inflammation in Human ISG15 Deficiency Leads to Necrotizing Skin Lesions. <i>Cell Reports</i> , 2020, 31, 107633.	6.4	47
15	The Underlying Mechanism of HNO Production by the Myoglobin-Mediated Oxidation of Hydroxylamine. <i>Inorganic Chemistry</i> , 2020, 59, 7939-7952.	4.0	7
16	Aromatic clusters in protein-protein and protein-drug complexes. <i>Journal of Cheminformatics</i> , 2020, 12, 30.	6.1	38
17	Structure and function of crocodilian hemoglobins and allosteric regulation by chloride, ATP, and CO <sub>2</sub> . <i>American Journal of Physiology - Regulatory Integrative and Comparative Physiology</i> , 2020, 318, R657-R667.	1.8	12
18	Reaction of Amines with NO at room temperature and atmospheric pressure: is nitroxyl a reaction intermediate?. <i>Pure and Applied Chemistry</i> , 2020, 92, 2005-2014.	1.9	3

#	ARTICLE	IF	CITATIONS
19	Spastic ataxia with eye-of-the-tiger-like sign in 4 siblings due to novel compound heterozygous AFG3L2 mutation. <i>Parkinsonism and Related Disorders</i> , 2020, 73, 52-54.	2.2	7
20	Integrating Omics Data to Prioritize Target Genes in Pathogenic Bacteria. <i>Computational Biology</i> , 2020, , 217-276.	0.2	1
21	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
22	AutoDock Bias: improving binding mode prediction and virtual screening using known protein-ligand interactions. <i>Bioinformatics</i> , 2019, 35, 3836-3838.	4.1	42
23	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
24	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
25	An efficient use of X-ray information, homology modeling, molecular dynamics and knowledge-based docking techniques to predict protein-monosaccharide complexes. <i>Glycobiology</i> , 2019, 29, 124-136.	2.5	8
26	Evaluation of nitroxyl donors' effect on mycobacteria. <i>Tuberculosis</i> , 2018, 109, 35-40.	1.9	8
27	Target-Pathogen: a structural bioinformatic approach to prioritize drug targets in pathogens. <i>Nucleic Acids Research</i> , 2018, 46, D413-D418.	14.5	53
28	Structural and mechanistic comparison of the Cyclopropane Mycolic Acid Synthases (CMAS) protein family of <i>Mycobacterium tuberculosis</i> . <i>Biochemical and Biophysical Research Communications</i> , 2018, 498, 288-295.	2.1	8
29	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
30	VarQ: A Tool for the Structural and Functional Analysis of Human Protein Variants. <i>Frontiers in Genetics</i> , 2018, 9, 620.	2.3	10
31	Solvents to Fragments to Drugs: MD Applications in Drug Design. <i>Molecules</i> , 2018, 23, 3269.	3.8	25
32	Reactive nitrogen and oxygen species: Friend or foe in the tuberculosis fight. <i>Tuberculosis</i> , 2018, 113, 175-176.	1.9	2
33	An optimized methodology for whole genome sequencing of RNA respiratory viruses from nasopharyngeal aspirates. <i>PLoS ONE</i> , 2018, 13, e0199714.	2.5	30
34	Genetics and genomic medicine in Argentina. <i>Molecular Genetics &amp; Genomic Medicine</i> , 2018, 6, 481-491.	1.2	17
35	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
36	Next generation sequencing panel based on single molecule molecular inversion probes for detecting genetic variants in children with hypopituitarism. <i>Molecular Genetics &amp; Genomic Medicine</i> , 2018, 6, 514-525.	1.2	17

#	ARTICLE	IF	CITATIONS
37	Single nucleotide polymorphisms may explain the contrasting phenotypes of two variants of a multidrug-resistant Mycobacterium tuberculosis strain. Tuberculosis, 2017, 103, 28-36.	1.9	10
38	Tyrosine oxidation and nitration in transmembrane peptides is connected to lipid peroxidation. Archives of Biochemistry and Biophysics, 2017, 622, 9-25.	3.0	14
39	Molecular Dynamics in Mixed Solvents Reveals Protein-Ligand Interactions, Improves Docking, and Allows Accurate Binding Free Energy Predictions. Journal of Chemical Information and Modeling, 2017, 57, 846-863.	5.4	68
40	Theoretical Insights into the Reaction and Inhibition Mechanism of Metal-Independent Retaining Glycosyltransferase Responsible for Mycothiol Biosynthesis. Journal of Physical Chemistry B, 2017, 121, 471-478.	2.6	9
41	HNO Is Produced by the Reaction of NO with Thiols. Journal of the American Chemical Society, 2017, 139, 14483-14487.	13.7	41
42	Tertiary and quaternary structural basis of oxygen affinity in human hemoglobin as revealed by multiscale simulations. Scientific Reports, 2017, 7, 10926.	3.3	23
43	LigQ: A Webserver to Select and Prepare Ligands for Virtual Screening. Journal of Chemical Information and Modeling, 2017, 57, 1741-1746.	5.4	5
44	Germline and somatic mutations in cortical malformations: Molecular defects in Argentinean patients with neuronal migration disorders. PLoS ONE, 2017, 12, e0185103.	2.5	20
45	Heme oxygenase-1 in the forefront of a multi-molecular network that governs cell-cell contacts and filopodia-induced zippering in prostate cancer. Cell Death and Disease, 2016, 7, e2570-e2570.	6.3	30
46	Mechanism of the Reaction of Human Manganese Superoxide Dismutase with Peroxynitrite: Nitration of Critical Tyrosine 34. Biochemistry, 2016, 55, 3403-3417.	2.5	37
47	Structural Study of a Flexible Active Site Loop in Human Indoleamine 2,3-Dioxygenase and Its Functional Implications. Biochemistry, 2016, 55, 2785-2793.	2.5	21
48	Binding of the substrate UDP-glucuronic acid induces conformational changes in the xanthan gum glucuronosyltransferase. Protein Engineering, Design and Selection, 2016, 29, 197-207.	2.1	5
49	Coarse-Grained Simulations of Heme Proteins: Validation and Study of Large Conformational Transitions. Journal of Chemical Theory and Computation, 2016, 12, 3390-3397.	5.3	10
50	Allelic differences in a vacuolar invertase affect Arabidopsis growth at early plant development. Journal of Experimental Botany, 2016, 67, 4091-4103.	4.8	20
51	Rapid Whole-Cell Assay of Antitubercular Drugs Using Second-Generation Fluoromycobacteriophages. Antimicrobial Agents and Chemotherapy, 2016, 60, 3253-3256.	3.2	13
52	A quantitative model for oxygen uptake and release in a family of heme proteins. Bioinformatics, 2016, 32, 1805-1813.	4.1	15
53	Structural Insights into the HWE Histidine Kinase Family: The Brucella Blue Light-Activated Histidine Kinase Domain. Journal of Molecular Biology, 2016, 428, 1165-1179.	4.2	18
54	A whole genome bioinformatic approach to determine potential latent phase specific targets in Mycobacterium tuberculosis. Tuberculosis, 2016, 97, 181-192.	1.9	21

#	ARTICLE	IF	CITATIONS
55	CG2AA: backmapping protein coarse-grained structures. <i>Bioinformatics</i> , 2016, 32, 1235-1237.	4.1	59
56	Evolutionary and Functional Relationships in the Truncated Hemoglobin Family. <i>PLoS Computational Biology</i> , 2016, 12, e1004701.	3.2	36
57	Whole Genome Sequencing Reveals a De Novo SHANK3 Mutation in Familial Autism Spectrum Disorder. <i>PLoS ONE</i> , 2015, 10, e0116358.	2.5	55
58	Molecular Mechanism of Myoglobin Autoxidation: Insights from Computer Simulations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1802-1813.	2.6	23
59	WATCLUST: a tool for improving the design of drugs based on protein-water interactions. <i>Bioinformatics</i> , 2015, 31, 3697-3699.	4.1	47
60	Efficient Calculation of Enzyme Reaction Free Energy Profiles Using a Hybrid Differential Relaxation Algorithm. <i>Advances in Protein Chemistry and Structural Biology</i> , 2015, 100, 33-65.	2.3	5
61	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
62	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
63	Discussing Endogenous NO $\leftrightarrow$ HNO Interconversion Aided by Phenolic Drugs and Vitamins. <i>Inorganic Chemistry</i> , 2015, 54, 9342-9350.	4.0	36
64	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
65	Using crystallographic water properties for the analysis and prediction of lectin-carbohydrate complex structures. <i>Glycobiology</i> , 2015, 25, 181-196.	2.5	19
66	Ligand uptake in Mycobacterium tuberculosis truncated hemoglobins is controlled by both internal tunnels and active site water molecules. <i>F1000Research</i> , 2015, 4, 22.	1.6	8
67	Ligand uptake in Mycobacterium tuberculosis truncated hemoglobins is controlled by both internal tunnels and active site water molecules. <i>F1000Research</i> , 2015, 4, 22.	1.6	11
68	Mechanistic Insight into the Enzymatic Reduction of Truncated Hemoglobin N of Mycobacterium tuberculosis. <i>Journal of Biological Chemistry</i> , 2014, 289, 21573-21583.	3.4	15
69	TuberQ: a Mycobacterium tuberculosis protein druggability database. <i>Database: the Journal of Biological Databases and Curation</i> , 2014, 2014, bau035-bau035.	3.0	35
70	QM/MM study of the C $\rightarrow$ 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
71	Underlying Thermodynamics of pH-Dependent Allostery. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12818-12826.	2.6	26
72	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

#	ARTICLE	IF	CITATIONS
73	H2S and NO cooperatively regulate vascular tone by activating a neuroendocrine HNO $\alpha$ -TRPA1 $\alpha$ -CGRP signalling pathway. <i>Nature Communications</i> , 2014, 5, 4381.	12.8	324
74	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
75	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
76	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
77	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
78	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
79	Time-Resolved Electrochemical Quantification of Azanone (HNO) at Low Nanomolar Level. <i>Analytical Chemistry</i> , 2013, 85, 10262-10269.	6.5	73
80	Solvent structure improves docking prediction in lectin $\alpha$ -carbohydrate complexes. <i>Glycobiology</i> , 2013, 23, 241-258.	2.5	47
81	Hydrophobic Effect Drives Oxygen Uptake in Myoglobin via Histidine E7. <i>Journal of Biological Chemistry</i> , 2013, 288, 6754-6762.	3.4	28
82	Small ligand $\alpha$ -globin interactions: Reviewing lessons derived from computer simulation. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2013, 1834, 1722-1738.	2.3	37
83	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
84	The allosteric modulation of thyroxine-binding globulin affinity is entropy driven. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2013, 1830, 3570-3577.	2.4	3
85	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
86	pH-Dependent Conformational Changes in Proteins and Their Effect on Experimental pKas: The Case of Nitrophorin 4. <i>PLoS Computational Biology</i> , 2012, 8, e1002761.	3.2	110
87	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
88	Molecular basis of intramolecular electron transfer in proteins during radical-mediated oxidations: Computer simulation studies in model tyrosine $\alpha$ -cysteine peptides in solution. <i>Archives of Biochemistry and Biophysics</i> , 2012, 525, 82-91.	3.0	31
89	<sup>1</sup> H, <sup>15</sup> N and <sup>13</sup> C chemical shift assignments of the BA42 protein of the psychrophilic bacteria <i>Bizionia argentinensis</i> sp. nov. <i>Biomolecular NMR Assignments</i> , 2012, 6, 181-183.	0.8	3
90	Azanone (HNO) interaction with Heme proteins and metalloporphyrins. <i>Advances in Inorganic Chemistry</i> , 2012, , 97-139.	1.0	8

#	ARTICLE	IF	CITATIONS
91	CDK2 and PKA Mediated-Sequential Phosphorylation Is Critical for p19INK4d Function in the DNA Damage Response. PLoS ONE, 2012, 7, e35638.	2.5	19
92	Role of PheE15 Gate in Ligand Entry and Nitric Oxide Detoxification Function of Mycobacterium tuberculosis Truncated Hemoglobin N. PLoS ONE, 2012, 7, e49291.	2.5	26
93	The NtrY/X two-component system of <i>Brucella</i> spp. acts as a redox sensor and regulates the expression of nitrogen respiration enzymes. Molecular Microbiology, 2012, 85, 39-50.	2.5	72
94	Electron transfer dynamics of Rhodothermus marinus caa3 cytochrome c domains on biomimetic films. Physical Chemistry Chemical Physics, 2011, 13, 18088.	2.8	12
95	Ligand Migration in Methanosarcina acetivorans Protoglobin: Effects of Ligand Binding and Dimeric Assembly. Journal of Physical Chemistry B, 2011, 115, 13771-13780.	2.6	31
96	An Integrated Computational Analysis of the Structure, Dynamics, and Ligand Binding Interactions of the Human Galectin Network. Journal of Chemical Information and Modeling, 2011, 51, 1918-1930.	5.4	23
97	Role of the Distal Hydrogen-Bonding Network in Regulating Oxygen Affinity in the Truncated Hemoglobin III from Campylobacter jejuni. Biochemistry, 2011, 50, 3946-3956.	2.5	23
98	p38 $\beta$ Activation Triggers Dynamical Changes in Allosteric Docking Sites. Biochemistry, 2011, 50, 1384-1395.	2.5	11
99	Molecular Basis for the Substrate Stereoselectivity in Tryptophan Dioxygenase. Biochemistry, 2011, 50, 10910-10918.	2.5	42
100	Exploring the molecular basis of human manganese superoxide dismutase inactivation mediated by tyrosine 34 nitration. Archives of Biochemistry and Biophysics, 2011, 507, 304-309.	3.0	48
101	Structural Model for p75NTR-TrkA Intracellular Domain Interaction: A Combined FRET and Bioinformatics Study. Journal of Molecular Biology, 2011, 414, 681-698.	4.2	26
102	Aromatic-Aromatic Interactions in Proteins: Beyond the Dimer. Journal of Chemical Information and Modeling, 2011, 51, 1623-1633.	5.4	115
103	Nitroxyl (azanone) trapping by metalloporphyrins. Coordination Chemistry Reviews, 2011, 255, 2764-2784.	18.8	84
104	The peculiar heme pocket of the 2/2 hemoglobin of cold-adapted Pseudoalteromonas haloplanktis TAC125. Journal of Biological Inorganic Chemistry, 2011, 16, 299-311.	2.6	21
105	Biological activity and ligand binding mode to the progesterone receptor of A-homo analogues of progesterone. Bioorganic and Medicinal Chemistry, 2011, 19, 1683-1691.	3.0	6
106	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> . IUBMB Life, 2011, 63, 175-182.	3.4	14
107	Comparing and combining implicit ligand sampling with multiple steered molecular dynamics to study ligand migration processes in heme proteins. Journal of Computational Chemistry, 2011, 32, 2219-2231.	3.3	39
108	Structural basis for ligand recognition in a mushroom lectin: solvent structure as specificity predictor. Carbohydrate Research, 2011, 346, 939-948.	2.3	23

#	ARTICLE	IF	CITATIONS
109	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
110	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
111	Draft Genome Sequence of <i>Bizonia argentinensis</i> , Isolated from Antarctic Surface Water. <i>Journal of Bacteriology</i> , 2011, 193, 6797-6798.	2.2	12
112	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
113	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
114	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
115	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
116	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
117	Substrate stereospecificity in tryptophan dioxygenase and indoleamine 2,3-dioxygenase. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 2961-2972.	2.6	35
118	Insights on Glucocorticoid Receptor Activity Modulation through the Binding of Rigid Steroids. <i>PLoS ONE</i> , 2010, 5, e13279.	2.5	44
119	Stabilization and detection of nitroxyl by iron and cobalt porphyrins in solution and on surfaces. <i>Journal of Porphyrins and Phthalocyanines</i> , 2010, 14, 1012-1018.	0.8	4
120	Comparative Studies of Human Indoleamine 2,3-dioxygenase and Tryptophan Dioxygenase. , 2010, , .		1
121	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
122	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
123	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
124	Molecular Basis of Coupled Protein and Electron Transfer Dynamics of Cytochrome c in Biomimetic Complexes. <i>Journal of the American Chemical Society</i> , 2010, 132, 5769-5778.	13.7	64
125	Linking the Structure and Thermal Stability of $\beta^2$ -Galactoside-Binding Protein Galectin-1 to Ligand Binding and Dimerization Equilibria. <i>Biochemistry</i> , 2010, 49, 7652-7658.	2.5	18
126	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

#	ARTICLE	IF	CITATIONS
127	Evidence for a ferryl intermediate in a heme-based dioxygenase. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 17371-17376.	7.1	113
128	Computer simulation and SERR detection of cytochrome c dynamics at SAM-coated electrodes. Electrochimica Acta, 2009, 54, 4963-4970.	5.2	32
129	High pressure reveals structural determinants for globin hexacoordination: Neuroglobin and myoglobin cases. Proteins: Structure, Function and Bioinformatics, 2009, 75, 885-894.	2.6	43
130	The hemoglobins of the sub-Antarctic fish <i>Cottoperca gobio</i> , a phylogenetically basal species oxygen-binding equilibria, kinetics and molecular dynamics. FEBS Journal, 2009, 276, 2266-2277.	4.7	27
131	Molecular Basis for the Electric Field Modulation of Cytochrome <i>c</i> Structure and Function. Journal of the American Chemical Society, 2009, 131, 16248-16256.	13.7	66
132	Thyroid Hormone Interactions with DMPC Bilayers. A Molecular Dynamics Study. Journal of Physical Chemistry B, 2009, 113, 13357-13364.	2.6	8
133	Molecular Basis for the pH Dependent Structural Transition of Nitrophorin 4. Journal of Physical Chemistry B, 2009, 113, 2135-2142.	2.6	19
134	pH-Dependent Mechanism of Nitric Oxide Release in Nitrophorins 2 and 4. Journal of Physical Chemistry B, 2009, 113, 1192-1201.	2.6	37
135	Carbohydrate-Binding Proteins: Dissecting Ligand Structures through Solvent Environment Occupancy. Journal of Physical Chemistry B, 2009, 113, 8717-8724.	2.6	33
136	Exploring the molecular basis of heme coordination in human neuroglobin. Proteins: Structure, Function and Bioinformatics, 2008, 71, 695-705.	2.6	54
137	Structural determinants of ligand migration in <i>Mycobacterium tuberculosis</i> truncated hemoglobin O. Proteins: Structure, Function and Bioinformatics, 2008, 73, 372-379.	2.6	47
138	Hemisuccinate of 21-Hydroxy-19-Epoxyprogesterone: A Tissue-Specific Modulator of the Glucocorticoid Receptor. ChemMedChem, 2008, 3, 1869-1877.	3.2	16
139	The role of residue Thr122 of methylamine dehydrogenase on the proton transfer from the iminoquinone intermediate to residue Asp76. Chemical Physics Letters, 2008, 456, 243-246.	2.6	2
140	Nitric Oxide Reactivity with Globins as Investigated Through Computer Simulation. Methods in Enzymology, 2008, 437, 477-498.	1.0	26
141	Bond or Cage Effect: How Nitrophorins Transport and Release Nitric Oxide. Journal of the American Chemical Society, 2008, 130, 1611-1618.	13.7	38
142	A Microscopic Study of the Deoxyhemoglobin-Catalyzed Generation of Nitric Oxide from Nitrite Anion. Biochemistry, 2008, 47, 9793-9802.	2.5	62
143	Trapping and Characterization of a Reaction Intermediate in Carbapenem Hydrolysis by <i>B. cereus</i> Metallo- $\beta$ -lactamase. Journal of the American Chemical Society, 2008, 130, 15852-15863.	13.7	72
144	Mechanism of Product Release in NO Detoxification from <i>Mycobacterium tuberculosis</i> Truncated Hemoglobin N. Journal of the American Chemical Society, 2008, 130, 1688-1693.	13.7	35

#	ARTICLE	IF	CITATIONS
145	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
146	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
147	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
148	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
149	HNO trapping and assisted decomposition of nitroxyl donors by ferric hemes. <i>Polyhedron</i> , 2007, 26, 4673-4679.	2.2	35
150	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
151	Modeling heme proteins using atomistic simulations. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 5611-5628.	2.8	77
152	The Catalytic Mechanism of Peptidylglycine Î±-Hydroxylating Monooxygenase Investigated by Computer Simulation. <i>Journal of the American Chemical Society</i> , 2006, 128, 12817-12828.	13.7	137
153	Ligand-induced dynamical regulation of NO conversion in <i>Mycobacterium tuberculosis</i> truncated hemoglobin-N. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 64, 457-464.	2.6	95
154	Dioxygen affinity in heme proteins investigated by computer simulation. <i>Journal of Inorganic Biochemistry</i> , 2006, 100, 761-770.	3.5	89
155	Free Energy Calculations with Non-Equilibrium Methods: Applications of the Jarzynski Relationship. <i>Theoretical Chemistry Accounts</i> , 2006, 116, 338-346.	1.4	79
156	Heme Protein Oxygen Affinity Regulation Exerted by Proximal Effects. <i>Journal of the American Chemical Society</i> , 2006, 128, 12455-12461.	13.7	91
157	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
158	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
159	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
160	Nitric Oxide Interaction with Cytochrome c 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
161	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
162	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

#	ARTICLE	IF	CITATIONS
163	QM-MM Study of Nitrite Reduction by Nitrite Reductase of <i>Pseudomonas aeruginosa</i> . Journal of Physical Chemistry B, 2004, 108, 18073-18080.	2.6	39
164	Modulation of the NO trans effect in heme proteins: implications for the activation of soluble guanylate cyclase. Journal of Biological Inorganic Chemistry, 2003, 8, 595-600.	2.6	39
165	Fast Nitroxyl Trapping by Ferric Porphyrins. Journal of the American Chemical Society, 2003, 125, 15272-15273.	13.7	82
166	A DFT-Based QM-MM Approach Designed for the Treatment of Large Molecular Systems: Application to Chorismate Mutase. Journal of Physical Chemistry B, 2003, 107, 13728-13736.	2.6	116
167	Physiological concentrations of melatonin inhibit the nitridergic pathway in the Syrian hamster retina. Journal of Pineal Research, 2002, 33, 31-36.	7.4	47
168	Environment effects on chemical reactivity of heme proteins. International Journal of Quantum Chemistry, 2002, 90, 1505-1514.	2.0	23
169	Cosolvent Sites-Based Discovery of <i>Mycobacterium Tuberculosis</i> Protein Kinase G Inhibitors. Journal of Medicinal Chemistry, 0, , .	6.4	3