

# Marcelo A Marti

## List of Publications by Year in Descending Order

**Source:** <https://exaly.com/author-pdf/6181792/marcelo-a-marti-publications-by-year.pdf>

**Version:** 2024-04-28

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

170  
papers

5,029  
citations

40  
h-index

59  
g-index

178  
ext. papers

5,668  
ext. citations

5.9  
avg, IF

5.35  
L-index

#	Paper	IF	Citations
170	MotSAsi: Functional short linear motifs (SLiMs) prediction based on genomic single nucleotide variants and structural data.. <i>Biochimie</i> , <b>2022</b> , 197, 59-73	4.6	0
169	Pulmonary Alveolar Proteinosis and Multiple Infectious Diseases in a Child with Autosomal Recessive Complete IRF8 Deficiency.. <i>Journal of Clinical Immunology</i> , <b>2022</b> , 1	5.7	0
168	Mycobacterium tuberculosis DosS binds HS through its Fe heme iron to regulate the DosR dormancy regulon.. <i>Redox Biology</i> , <b>2022</b> , 52, 102316	11.3	0
167	A Remote Secondary Binding Pocket Promotes Heteromultivalent Targeting of DC-SIGN. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 18977-18988	16.4	2
166	Clamping, bending, and twisting inter-domain motions in the misfold-recognizing portion of UDP-glucose: Glycoprotein glucosyltransferase. <i>Structure</i> , <b>2021</b> , 29, 357-370.e9	5.2	5
165	From Genome to Drugs: New Approaches in Antimicrobial Discovery. <i>Frontiers in Pharmacology</i> , <b>2021</b> , 12, 647060	5.6	1
164	Structural modeling of a novel membrane-bound globin-coupled sensor in. <i>Computational and Structural Biotechnology Journal</i> , <b>2021</b> , 19, 1874-1888	6.8	0
163	Oculocutaneous albinism type 1B associated with a functionally significant tyrosinase gene polymorphism detected with Whole Exome Sequencing. <i>Ophthalmic Genetics</i> , <b>2021</b> , 42, 291-295	1.2	0
162	High-throughput splicing assays identify missense and silent splice-disruptive POU1F1 variants underlying pituitary hormone deficiency. <i>American Journal of Human Genetics</i> , <b>2021</b> , 108, 1526-1539	11	5
161	Biased Docking for Protein-Ligand Pose Prediction. <i>Methods in Molecular Biology</i> , <b>2021</b> , 2266, 39-72	1.4	2
160	Systemic Type I IFN Inflammation in Human ISG15 Deficiency Leads to Necrotizing Skin Lesions. <i>Cell Reports</i> , <b>2020</b> , 31, 107633	10.6	19
159	The Underlying Mechanism of HNO Production by the Myoglobin-Mediated Oxidation of Hydroxylamine. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 7939-7952	5.1	6
158	Aromatic clusters in protein-protein and protein-drug complexes. <i>Journal of Cheminformatics</i> , <b>2020</b> , 12, 30	8.6	6
157	Structure and function of crocodilian hemoglobins and allosteric regulation by chloride, ATP, and CO. <i>American Journal of Physiology - Regulatory Integrative and Comparative Physiology</i> , <b>2020</b> , 318, R657-R667	3.2	6
156	Reaction of Amines with NO at room temperature and atmospheric pressure: is nitroxyl a reaction intermediate?. <i>Pure and Applied Chemistry</i> , <b>2020</b> , 92, 2005-2014	2.1	3
155	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> , <b>2020</b> , 73, 52-54	3.6	3
154	Integrating Omics Data to Prioritize Target Genes in Pathogenic Bacteria. <i>Computational Biology</i> , <b>2020</b> , 217-276	0.7	1

153	Conformational and Reaction Dynamic Coupling in Histidine Kinases: Insights from Hybrid QM/MM Simulations. <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 833-842	6.1	4
152	Kinase Activation by Small Conformational Changes. <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 821-832	6.1	6
151	AutoDock Bias: improving binding mode prediction and virtual screening using known protein-ligand interactions. <i>Bioinformatics</i> , <b>2019</b> , 35, 3836-3838	7.2	22
150	Cosolvent-Based Protein Pharmacophore for Ligand Enrichment in Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 3572-3583	6.1	11
149	The Structural Biology of Galectin-Ligand Recognition: Current Advances in Modeling Tools, Protein Engineering, and Inhibitor Design. <i>Frontiers in Chemistry</i> , <b>2019</b> , 7, 823	5	35
148	Gordon Holmes Syndrome Caused by RNF216 Novel Mutation in 2 Argentinean Siblings. <i>Movement Disorders Clinical Practice</i> , <b>2019</b> , 6, 259-262	2.2	7
147	An efficient use of X-ray information, homology modeling, molecular dynamics and knowledge-based docking techniques to predict protein-monosaccharide complexes. <i>Glycobiology</i> , <b>2019</b> , 29, 124-136	5.8	5
146	Evaluation of nitroxyl donors effect on mycobacteria. <i>Tuberculosis</i> , <b>2018</b> , 109, 35-40	2.6	8
145	Target-Pathogen: a structural bioinformatic approach to prioritize drug targets in pathogens. <i>Nucleic Acids Research</i> , <b>2018</b> , 46, D413-D418	20.1	29
144	Structural and mechanistic comparison of the Cyclopropane Mycolic Acid Synthases (CMAS) protein family of Mycobacterium tuberculosis. <i>Biochemical and Biophysical Research Communications</i> , <b>2018</b> , 498, 288-295	3.4	6
143	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> , <b>2018</b> , 498, 305-312	3.4	6
142	Genetics and genomic medicine in Argentina. <i>Molecular Genetics &amp; Genomic Medicine</i> , <b>2018</b> , 6, 481	2.3	13
141	An integrative, multi-omics approach towards the prioritization of Klebsiella pneumoniae drug targets. <i>Scientific Reports</i> , <b>2018</b> , 8, 10755	4.9	28
140	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> , <b>2018</b> , 6, 514	2.3	12
139	VarQ: A Tool for the Structural and Functional Analysis of Human Protein Variants. <i>Frontiers in Genetics</i> , <b>2018</b> , 9, 620	4.5	6
138	Solvents to Fragments to Drugs: MD Applications in Drug Design. <i>Molecules</i> , <b>2018</b> , 23,	4.8	14
137	Reactive nitrogen and oxygen species: Friend or foe in the tuberculosis fight. <i>Tuberculosis</i> , <b>2018</b> , 113, 175-176	2.6	2
136	An optimized methodology for whole genome sequencing of RNA respiratory viruses from nasopharyngeal aspirates. <i>PLoS ONE</i> , <b>2018</b> , 13, e0199714	3.7	19

135	Single nucleotide polymorphisms may explain the contrasting phenotypes of two variants of a multidrug-resistant <i>Mycobacterium tuberculosis</i> strain. <i>Tuberculosis</i> , <b>2017</b> , 103, 28-36	2.6	10
134	Tyrosine oxidation and nitration in transmembrane peptides is connected to lipid peroxidation. <i>Archives of Biochemistry and Biophysics</i> , <b>2017</b> , 622, 9-25	4.1	9
133	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> , <b>2017</b> , 57, 846-863	6.1	43
132	Theoretical Insights into the Reaction and Inhibition Mechanism of Metal-Independent Retaining Glycosyltransferase Responsible for Mycothiol Biosynthesis. <i>Journal of Physical Chemistry B</i> , <b>2017</b> , 121, 471-478	3.4	6
131	Germline and somatic mutations in cortical malformations: Molecular defects in Argentinean patients with neuronal migration disorders. <i>PLoS ONE</i> , <b>2017</b> , 12, e0185103	3.7	14
130	HNO Is Produced by the Reaction of NO with Thiols. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 14483-14487	16.4	33
129	Tertiary and quaternary structural basis of oxygen affinity in human hemoglobin as revealed by multiscale simulations. <i>Scientific Reports</i> , <b>2017</b> , 7, 10926	4.9	13
128	LigQ: A Webserver to Select and Prepare Ligands for Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 1741-1746	6.1	4
127	Coarse-Grained Simulations of Heme Proteins: Validation and Study of Large Conformational Transitions. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 3390-7	6.4	8
126	Allelic differences in a vacuolar invertase affect Arabidopsis growth at early plant development. <i>Journal of Experimental Botany</i> , <b>2016</b> , 67, 4091-103	7	12
125	Rapid Whole-Cell Assay of Antitubercular Drugs Using Second-Generation Fluoromycobacteriophages. <i>Antimicrobial Agents and Chemotherapy</i> , <b>2016</b> , 60, 3253-6	5.9	9
124	A quantitative model for oxygen uptake and release in a family of heme proteins. <i>Bioinformatics</i> , <b>2016</b> , 32, 1805-13	7.2	12
123	Structural Insights into the HWE Histidine Kinase Family: The Brucella Blue Light-Activated Histidine Kinase Domain. <i>Journal of Molecular Biology</i> , <b>2016</b> , 428, 1165-1179	6.5	13
122	A whole genome bioinformatic approach to determine potential latent phase specific targets in <i>Mycobacterium tuberculosis</i> . <i>Tuberculosis</i> , <b>2016</b> , 97, 181-92	2.6	15
121	CG2AA: backmapping protein coarse-grained structures. <i>Bioinformatics</i> , <b>2016</b> , 32, 1235-7	7.2	32
120	Evolutionary and Functional Relationships in the Truncated Hemoglobin Family. <i>PLoS Computational Biology</i> , <b>2016</b> , 12, e1004701	5	23
119	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> , <b>2016</b> , 7, e2570	9.8	23
118	Mechanism of the Reaction of Human Manganese Superoxide Dismutase with Peroxynitrite: Nitration of Critical Tyrosine 34. <i>Biochemistry</i> , <b>2016</b> , 55, 3403-17	3.2	32

117	Structural Study of a Flexible Active Site Loop in Human Indoleamine 2,3-Dioxygenase and Its Functional Implications. <i>Biochemistry</i> , <b>2016</b> , 55, 2785-93	3.2	20
116	Binding of the substrate UDP-glucuronic acid induces conformational changes in the xanthan gum glucuronosyltransferase. <i>Protein Engineering, Design and Selection</i> , <b>2016</b> , 29, 197-207	1.9	4
115	Molecular mechanism of myoglobin autoxidation: insights from computer simulations. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 1802-13	3.4	19
114	WATCLUST: a tool for improving the design of drugs based on protein-water interactions. <i>Bioinformatics</i> , <b>2015</b> , 31, 3697-9	7.2	35
113	Efficient Calculation of Enzyme Reaction Free Energy Profiles Using a Hybrid Differential Relaxation Algorithm: Application to Mycobacterial Zinc Hydrolases. <i>Advances in Protein Chemistry and Structural Biology</i> , <b>2015</b> , 100, 33-65	5.3	4
112	Protein topology determines cysteine oxidation fate: the case of sulfenyl amide formation among protein families. <i>PLoS Computational Biology</i> , <b>2015</b> , 11, e1004051	5	34
111	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> , <b>2015</b> , 137, 4720-7	16.4	64
110	Discussing endogenous NO( $\rightleftharpoons$ )HNO interconversion aided by phenolic drugs and vitamins. <i>Inorganic Chemistry</i> , <b>2015</b> , 54, 9342-50	5.1	31
109	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> , <b>2015</b> , 1850, 169-77	4	15
108	Using crystallographic water properties for the analysis and prediction of lectin-carbohydrate complex structures. <i>Glycobiology</i> , <b>2015</b> , 25, 181-96	5.8	13
107	Whole genome sequencing reveals a de novo SHANK3 mutation in familial autism spectrum disorder. <i>PLoS ONE</i> , <b>2015</b> , 10, e0116358	3.7	38
106	Ligand uptake in Mycobacterium tuberculosis truncated hemoglobins is controlled by both internal tunnels and active site water molecules. <i>F1000Research</i> , <b>2015</b> , 4, 22	3.6	8
105	Ligand uptake in Mycobacterium tuberculosis truncated hemoglobins is controlled by both internal tunnels and active site water molecules. <i>F1000Research</i> , <b>2015</b> , 4, 22	3.6	9
104	QM/MM study of the C-C coupling reaction mechanism of CYP121, an essential cytochrome p450 of Mycobacterium tuberculosis. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2014</b> , 82, 1004-21	4.2	20
103	Underlying thermodynamics of pH-dependent allostery. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 12818-26	3.4	23
102	Improving Efficiency in SMD Simulations Through a Hybrid Differential Relaxation Algorithm. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 4609-17	6.4	12
101	H <sub>2</sub> S and NO cooperatively regulate vascular tone by activating a neuroendocrine HNO-TRPA1-CGRP signalling pathway. <i>Nature Communications</i> , <b>2014</b> , 5, 4381	17.4	267
100	Reactions of HNO with metal porphyrins: underscoring the biological relevance of HNO. <i>Accounts of Chemical Research</i> , <b>2014</b> , 47, 2907-16	24.3	51

99	Structural and molecular basis of the peroxynitrite-mediated nitration and inactivation of Trypanosoma cruzi iron-superoxide dismutases (Fe-SODs) A and B: disparate susceptibilities due to the repair of Tyr35 radical by Cys83 in Fe-SODB through intramolecular electron transfer. <i>Journal of Biological Chemistry</i> , <b>2014</b> , 289, 12760-78	5-4	43
98	Redox potential determines the reaction mechanism of HNO donors with Mn and Fe porphyrins: defining the better traps. <i>Inorganic Chemistry</i> , <b>2014</b> , 53, 7351-60	5-1	33
97	How to Find an HNO Needle in a (Bio)-Chemical Haystack. <i>Progress in Inorganic Chemistry</i> , <b>2014</b> , 145-184		2
96	Mechanistic insight into the enzymatic reduction of truncated hemoglobin N of Mycobacterium tuberculosis: role of the CD loop and pre-A motif in electron cycling. <i>Journal of Biological Chemistry</i> , <b>2014</b> , 289, 21573-83	5-4	14
95	TuberQ: a Mycobacterium tuberculosis protein druggability database. <i>Database: the Journal of Biological Databases and Curation</i> , <b>2014</b> , 2014, bau035	5	24
94	Heme-oxygenase-1 implications in cell morphology and the adhesive behavior of prostate cancer cells. <i>Oncotarget</i> , <b>2014</b> , 5, 4087-102	3-3	42
93	Molecular Dynamics Simulations Provide Atomistic Insight into Hydrogen Exchange Mass Spectrometry Experiments. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 658-69	6-4	23
92	Time-resolved electrochemical quantification of azanone (HNO) at low nanomolar level. <i>Analytical Chemistry</i> , <b>2013</b> , 85, 10262-9	7-8	63
91	Solvent structure improves docking prediction in lectin-carbohydrate complexes. <i>Glycobiology</i> , <b>2013</b> , 23, 241-58	5-8	32
90	Hydrophobic effect drives oxygen uptake in myoglobin via histidine E7. <i>Journal of Biological Chemistry</i> , <b>2013</b> , 288, 6754-62	5-4	26
89	Small ligand-globin interactions: reviewing lessons derived from computer simulation. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , <b>2013</b> , 1834, 1722-38	4	32
88	Quaternary structure effects on the hexacoordination equilibrium in rice hemoglobin rHb1: insights from molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2013</b> , 81, 863-73	4-2	8
87	The allosteric modulation of thyroxine-binding globulin affinity is entropy driven. <i>Biochimica Et Biophysica Acta - General Subjects</i> , <b>2013</b> , 1830, 3570-7	4	3
86	The key role of water in the dioxygenase function of Escherichia coli flavohemoglobin. <i>Journal of Inorganic Biochemistry</i> , <b>2013</b> , 119, 75-84	4-2	9
85	The NtrY/X two-component system of Brucella spp. acts as a redox sensor and regulates the expression of nitrogen respiration enzymes. <i>Molecular Microbiology</i> , <b>2012</b> , 85, 39-50	4-1	44
84	Complete reaction mechanism of indoleamine 2,3-dioxygenase as revealed by QM/MM simulations. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 1401-13	3-4	62
83	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> , <b>2012</b> , 525, 82-91	4-1	29
82	<sup>1</sup> H, <sup>15</sup> N and <sup>13</sup> C chemical shift assignments of the BA42 protein of the psychrophilic bacteria Bizionia argentinensis sp. nov. <i>Biomolecular NMR Assignments</i> , <b>2012</b> , 6, 181-3	0-7	2

81	Azanone (HNO) interaction with Hemeproteins and metalloporphyrins. <i>Advances in Inorganic Chemistry</i> , <b>2012</b> , 97-139	2.1	7
80	CDK2 and PKA mediated-sequential phosphorylation is critical for p19INK4d function in the DNA damage response. <i>PLoS ONE</i> , <b>2012</b> , 7, e35638	3.7	17
79	Role of PheE15 gate in ligand entry and nitric oxide detoxification function of mycobacterium tuberculosis truncated hemoglobin N. <i>PLoS ONE</i> , <b>2012</b> , 7, e49291	3.7	25
78	pH-Dependent conformational changes in proteins and their effect on experimental pK(a)s: the case of Nitrophorin 4. <i>PLoS Computational Biology</i> , <b>2012</b> , 8, e1002761	5	90
77	Role of the distal hydrogen-bonding network in regulating oxygen affinity in the truncated hemoglobin III from <i>Campylobacter jejuni</i> . <i>Biochemistry</i> , <b>2011</b> , 50, 3946-56	3.2	23
76	p38 $\beta$ activation triggers dynamical changes in allosteric docking sites. <i>Biochemistry</i> , <b>2011</b> , 50, 1384-95	3.2	9
75	Molecular basis for the substrate stereoselectivity in tryptophan dioxygenase. <i>Biochemistry</i> , <b>2011</b> , 50, 10910-8	3.2	37
74	Exploring the molecular basis of human manganese superoxide dismutase inactivation mediated by tyrosine 34 nitration. <i>Archives of Biochemistry and Biophysics</i> , <b>2011</b> , 507, 304-9	4.1	45
73	Structural model for p75(NTR)-TrkA intracellular domain interaction: a combined FRET and bioinformatics study. <i>Journal of Molecular Biology</i> , <b>2011</b> , 414, 681-98	6.5	23
72	Aromatic-aromatic interactions in proteins: beyond the dimer. <i>Journal of Chemical Information and Modeling</i> , <b>2011</b> , 51, 1623-33	6.1	93
71	Nitroxyl (azanone) trapping by metalloporphyrins. <i>Coordination Chemistry Reviews</i> , <b>2011</b> , 255, 2764-2784	3.2	76
70	The peculiar heme pocket of the 2/2 hemoglobin of cold-adapted <i>Pseudoalteromonas haloplanktis</i> TAC125. <i>Journal of Biological Inorganic Chemistry</i> , <b>2011</b> , 16, 299-311	3.7	20
69	Biological activity and ligand binding mode to the progesterone receptor of A-homo analogues of progesterone. <i>Bioorganic and Medicinal Chemistry</i> , <b>2011</b> , 19, 1683-91	3.4	6
68	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> , <b>2011</b> , 63, 175-82	4.7	13
67	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> , <b>2011</b> , 32, 2219-315	3.5	39
66	Electron transfer dynamics of <i>Rhodothermus marinus</i> caa3 cytochrome c domains on biomimetic films. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 18088-98	3.6	12
65	Ligand migration in <i>Methanosarcina acetivorans</i> protoglobin: effects of ligand binding and dimeric assembly. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 13771-80	3.4	28
64	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> , <b>2011</b> , 51, 1918-30	6.1	21

63	Structural basis for ligand recognition in a mushroom lectin: solvent structure as specificity predictor. <i>Carbohydrate Research</i> , <b>2011</b> , 346, 939-48	2.9	19
62	Protein dynamics and ligand migration interplay as studied by computer simulation. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , <b>2011</b> , 1814, 1054-64	4	28
61	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> , <b>2011</b> , 105, 1044-9	4.2	18
60	Draft genome sequence of <i>Bizonia argentinensis</i> , isolated from Antarctic surface water. <i>Journal of Bacteriology</i> , <b>2011</b> , 193, 6797-8	3.5	9
59	Ligand migration in the apolar tunnel of <i>Cerebratulus lacteus</i> mini-hemoglobin. <i>Journal of Biological Chemistry</i> , <b>2011</b> , 286, 5347-58	5.4	20
58	Insights on glucocorticoid receptor activity modulation through the binding of rigid steroids. <i>PLoS ONE</i> , <b>2010</b> , 5, e13279	3.7	38
57	Stabilization and detection of nitroxyl by iron and cobalt porphyrins in solution and on surfaces. <i>Journal of Porphyrins and Phthalocyanines</i> , <b>2010</b> , 14, 1012-1018	1.8	3
56	Comparative Studies of Human Indoleamine 2,3-dioxygenase and Tryptophan Dioxygenase <b>2010</b> ,		1
55	A surface effect allows HNO/NO discrimination by a cobalt porphyrin bound to gold. <i>Inorganic Chemistry</i> , <b>2010</b> , 49, 6955-66	5.1	59
54	Role of heme distortion on oxygen affinity in heme proteins: the protoglobin case. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 8536-43	3.4	35
53	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> , <b>2010</b> , 114, 11251-60	3.4	13
52	Molecular basis of coupled protein and electron transfer dynamics of cytochrome c in biomimetic complexes. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 5769-78	16.4	61
51	Linking the structure and thermal stability of beta-galactoside-binding protein galectin-1 to ligand binding and dimerization equilibria. <i>Biochemistry</i> , <b>2010</b> , 49, 7652-8	3.2	15
50	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> , <b>2010</b> , 15, 811-23	3.7	47
49	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> , <b>2010</b> , 644, 138-45	5.3	48
48	Thermal fluctuations determine the electron-transfer rates of cytochrome c in electrostatic and covalent complexes. <i>ChemPhysChem</i> , <b>2010</b> , 11, 1225-35	3.2	34
47	Electron Transfer of Proteins at Membrane Models <b>2010</b> , 219-240		1
46	Unraveling the molecular basis for ligand binding in truncated hemoglobins: the trHbO <i>Bacillus subtilis</i> case. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2010</b> , 78, 962-70	4.2	35



45	Substrate stereo-specificity in tryptophan dioxygenase and indoleamine 2,3-dioxygenase. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2010</b> , 78, 2961-72	4.2	31
44	Role of Pre-A motif in nitric oxide scavenging by truncated hemoglobin, HbN, of Mycobacterium tuberculosis. <i>Journal of Biological Chemistry</i> , <b>2009</b> , 284, 14457-68	5.4	54
43	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> , <b>2009</b> , 106, 17371-6	11.5	101
42	Computer simulation and SERR detection of cytochrome c dynamics at SAM-coated electrodes. <i>Electrochimica Acta</i> , <b>2009</b> , 54, 4963-4970	6.7	30
41	High pressure reveals structural determinants for globin hexacoordination: neuroglobin and myoglobin cases. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2009</b> , 75, 885-94	4.2	40
40	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> , <b>2009</b> , 276, 2266-77	5.7	25
39	Molecular basis for the electric field modulation of cytochrome C structure and function. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 16248-56	16.4	49
38	Thyroid hormone interactions with DMPC bilayers. A molecular dynamics study. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 13357-64	3.4	8
37	Molecular basis for the pH dependent structural transition of Nitrophorin 4. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 2135-42	3.4	19
36	pH-dependent mechanism of nitric oxide release in nitrophorins 2 and 4. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 1192-201	3.4	35
35	Carbohydrate-binding proteins: Dissecting ligand structures through solvent environment occupancy. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 8717-24	3.4	30
34	Nitric oxide reactivity with globins as investigated through computer simulation. <i>Methods in Enzymology</i> , <b>2008</b> , 437, 477-98	1.7	24
33	Bond or cage effect: how nitrophorins transport and release nitric oxide. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 1611-8	16.4	37
32	A microscopic study of the deoxyhemoglobin-catalyzed generation of nitric oxide from nitrite anion. <i>Biochemistry</i> , <b>2008</b> , 47, 9793-802	3.2	59
31	Trapping and characterization of a reaction intermediate in carbapenem hydrolysis by <i>B. cereus</i> metallo-beta-lactamase. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 15852-63	16.4	65
30	Mechanism of product release in NO detoxification from Mycobacterium tuberculosis truncated hemoglobin N. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 1688-93	16.4	33
29	Dynamical characterization of the heme NO oxygen binding (HNOX) domain. Insight into soluble guanylate cyclase allosteric transition. <i>Biochemistry</i> , <b>2008</b> , 47, 9416-27	3.2	46
28	Exploring the molecular basis of action of the passive antiglucocorticoid 21-hydroxy-6,19-epoxyprogesterone. <i>Journal of Medicinal Chemistry</i> , <b>2008</b> , 51, 1352-60	8.3	21

27	Exploring the molecular basis of heme coordination in human neuroglobin. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2008</b> , 71, 695-705	4.2	51
26	Structural determinants of ligand migration in Mycobacterium tuberculosis truncated hemoglobin O. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2008</b> , 73, 372-9	4.2	46
25	Hemisuccinate of 21-hydroxy-6,19-epoxyprogesterone: a tissue-specific modulator of the glucocorticoid receptor. <i>ChemMedChem</i> , <b>2008</b> , 3, 1869-77	3.7	14
24	The role of residue Thr122 of methylamine dehydrogenase on the proton transfer from the iminoquinone intermediate to residue Asp76. <i>Chemical Physics Letters</i> , <b>2008</b> , 456, 243-246	2.5	2
23	Dynamical regulation of ligand migration by a gate-opening molecular switch in truncated hemoglobin-N from Mycobacterium tuberculosis. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 6782-8	16.4	42
22	HNO trapping and assisted decomposition of nitroxyl donors by ferric hemes. <i>Polyhedron</i> , <b>2007</b> , 26, 4673-4679	3.4	30
21	Oxygen affinity controlled by dynamical distal conformations: the soybean leghemoglobin and the Paramecium caudatum hemoglobin cases. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2007</b> , 68, 480-7	4.2	30
20	Characterization of the galectin-1 carbohydrate recognition domain in terms of solvent occupancy. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 7360-6	3.4	28
19	Free Energy Calculations with Non-Equilibrium Methods: Applications of the Jarzynski Relationship. <i>Theoretical Chemistry Accounts</i> , <b>2006</b> , 116, 338-346	1.9	65
18	Heme protein oxygen affinity regulation exerted by proximal effects. <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 12455-61	16.4	79
17	Modeling heme proteins using atomistic simulations. <i>Physical Chemistry Chemical Physics</i> , <b>2006</b> , 8, 5611-28	3.8	72
16	The catalytic mechanism of peptidylglycine alpha-hydroxylating monooxygenase investigated by computer simulation. <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 12817-28	16.4	126
15	Ligand-induced dynamical regulation of NO conversion in Mycobacterium tuberculosis truncated hemoglobin-N. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2006</b> , 64, 457-64	4.2	89
14	Dioxygen affinity in heme proteins investigated by computer simulation. <i>Journal of Inorganic Biochemistry</i> , <b>2006</b> , 100, 761-70	4.2	83
13	Two distinct heme distal site states define Cerebratulus lacteus mini-hemoglobin oxygen affinity. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2006</b> , 62, 641-8	4.2	20
12	Discrimination of nitroxyl and nitric oxide by water-soluble Mn(III) porphyrins. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 4680-4	16.4	102
11	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> , <b>2005</b> , 127, 7721-8	16.4	61
10	Theoretical study of the truncated hemoglobin HbN: exploring the molecular basis of the NO detoxification mechanism. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 4433-44	16.4	102

9	Multiple-steering QM-MM calculation of the free energy profile in chorismate mutase. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 6940-1	16.4	103
8	Proximal effects in the modulation of nitric oxide synthase reactivity: a QM-MM study. <i>Journal of Biological Inorganic Chemistry</i> , <b>2005</b> , 10, 595-604	3.7	14
7	QM-MM Study of Nitrite Reduction by Nitrite Reductase of <i>Pseudomonas aeruginosa</i> . <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 18073-18080	3.4	37
6	Modulation of the NO trans effect in heme proteins: implications for the activation of soluble guanylate cyclase. <i>Journal of Biological Inorganic Chemistry</i> , <b>2003</b> , 8, 595-600	3.7	39
5	Fast nitroxyl trapping by ferric porphyrins. <i>Journal of the American Chemical Society</i> , <b>2003</b> , 125, 15272-3	16.4	76
4	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> , <b>2003</b> , 107, 13728-13736	3.4	110
3	Physiological concentrations of melatonin inhibit the nitridergic pathway in the Syrian hamster retina. <i>Journal of Pineal Research</i> , <b>2002</b> , 33, 31-6	10.4	45
2	Environment effects on chemical reactivity of heme proteins. <i>International Journal of Quantum Chemistry</i> , <b>2002</b> , 90, 1505-1514	2.1	23
1	Clamping, bending, and twisting inter-domain motions in the misfold-recognising portion of UDP-glucose:glycoprotein glucosyl-transferase		1