

Claudio M. Soares

List of Publications by Year in descending order

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132
papers

5,780
citations

81889

39
h-index

88628

70
g-index

142
all docs

142
docs citations

142
times ranked

6435
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular and Biochemical Characterization of a Highly Stable Bacterial Laccase That Occurs as a Structural Component of the <i>Bacillus subtilis</i> Endospore Coat. <i>Journal of Biological Chemistry</i> , 2002, 277, 18849-18859.	3.4	456
2	Constant-pH molecular dynamics using stochastic titration. <i>Journal of Chemical Physics</i> , 2002, 117, 4184-4200.	3.0	283
3	Protein Structure and Dynamics in Ionic Liquids. Insights from Molecular Dynamics Simulation Studies. <i>Journal of Physical Chemistry B</i> , 2008, 112, 2566-2572.	2.6	199
4	[NiFe] hydrogenase from <i>Desulfovibrio desulfuricans</i> ATCC 27774: gene sequencing, three-dimensional structure determination and refinement at 1.8 Å... and modelling studies of its interaction with the tetrahaem cytochrome c 3. <i>Journal of Biological Inorganic Chemistry</i> , 2001, 6, 63-81.	2.6	198
5	Evolution of the Thyroid Hormone-Binding Protein, Transthyretin. <i>General and Comparative Endocrinology</i> , 2000, 119, 241-255.	1.8	182
6	Tailoring cutinase activity towards polyethylene terephthalate and polyamide 6,6 fibers. <i>Journal of Biotechnology</i> , 2007, 128, 849-857.	3.8	161
7	Ab initio determination of the crystal structure of cytochrome c6 and comparison with plastocyanin. <i>Structure</i> , 1995, 3, 1159-1169.	3.3	146
8	Sulphate respiration from hydrogen in <i>Desulfovibrio</i> bacteria: a structural biology overview. <i>Progress in Biophysics and Molecular Biology</i> , 2005, 89, 292-329.	2.9	141
9	Parametrization of 1-Butyl-3-methylimidazolium Hexafluorophosphate/Nitrate Ionic Liquid for the GROMOS Force Field. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14444-14451.	2.6	131
10	Mind the gap: cytochrome interactions reveal electron pathways across the periplasm of <i>Shewanella oneidensis</i> MR-1. <i>Biochemical Journal</i> , 2013, 449, 101-108.	3.7	129
11	Some Theoretical and Computational Aspects of the Inclusion of Proton Isomerism in the Protonation Equilibrium of Proteins. <i>Journal of Physical Chemistry B</i> , 2001, 105, 293-309.	2.6	122
12	Revertant mutants G550E and 4RK rescue cystic fibrosis mutants in the first nucleotide-binding domain of CFTR by different mechanisms. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 17891-17896.	7.1	112
13	Protein Structure and Dynamics in Nonaqueous Solvents: Insights from Molecular Dynamics Simulation Studies. <i>Biophysical Journal</i> , 2003, 84, 1628-1641.	0.5	110
14	Simulation of Electron-Proton Coupling with a Monte Carlo Method: Application to Cytochrome c3 Using Continuum Electrostatics. <i>Biophysical Journal</i> , 1999, 76, 2978-2998.	0.5	105
15	On the Use of Different Dielectric Constants for Computing Individual and Pairwise Terms in Poisson-Boltzmann Studies of Protein Ionization Equilibrium. <i>Journal of Physical Chemistry B</i> , 2005, 109, 14691-14706.	2.6	91
16	Nickel-Iron-Selenium Hydrogenases - An Overview. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 948-962.	2.0	86
17	Hydrogenases in <i>Desulfovibrio vulgaris</i> Hildenborough: structural and physiologic characterisation of the membrane-bound [NiFeSe] hydrogenase. <i>Journal of Biological Inorganic Chemistry</i> , 2005, 10, 667-682.	2.6	83
18	Crystal Structure of Cardosin A, a Glycosylated and Arg-Gly-Asp-containing Aspartic Proteinase from the Flowers of <i>Cynara cardunculus</i> L.. <i>Journal of Biological Chemistry</i> , 1999, 274, 27694-27701.	3.4	82

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19	Signatures in SARS-CoV-2 spike protein conferring escape to neutralizing antibodies. <i>PLoS Pathogens</i> , 2021, 17, e1009772.	4.7	74
20	Modeling hydration mechanisms of enzymes in nonpolar and polar organic solvents. <i>FEBS Journal</i> , 2007, 274, 2424-2436.	4.7	73
21	Mechanisms underlying dioxygen reduction in laccases. Structural and modelling studies focusing on proton transfer. <i>BMC Structural Biology</i> , 2010, 10, 28.	2.3	72
22	Improved modeling of side-chains in proteins with rotamer-based methods: A flexible rotamer model. , 1999, 37, 530-543.		68
23	Functional role of N-glycosylation from ADAM10 in processing, localization and activity of the enzyme. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2008, 1780, 905-913.	2.4	68
24	Pathways of H ₂ toward the Active Site of [NiFe]-Hydrogenase. <i>Biophysical Journal</i> , 2006, 91, 2035-2045.	0.5	66
25	Proximal mutations at the type I copper site of CotA laccase: spectroscopic, redox, kinetic and structural characterization of I494A and L386A mutants. <i>Biochemical Journal</i> , 2008, 412, 339-346.	3.7	66
26	Exploring the molecular mechanisms of electron shuttling across the microbe/metal space. <i>Frontiers in Microbiology</i> , 2014, 5, 318.	3.5	65
27	Electric-Field-Induced Redox Potential Shifts of Tetraheme Cytochromes c ₃ Immobilized on Self-Assembled Monolayers: Surface-Enhanced Resonance Raman Spectroscopy and Simulation Studies. <i>Biophysical Journal</i> , 2005, 88, 4188-4199.	0.5	63
28	Proton pathways in a [NiFe]-hydrogenase: A theoretical study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 1010-1022.	2.6	63
29	Studies of the reduction and protonation behavior of tetraheme cytochromes using atomic detail. <i>Journal of Biological Inorganic Chemistry</i> , 2002, 7, 200-216.	2.6	61
30	Conformational changes induced by ATP hydrolysis in an ABC transporter: A molecular dynamics study of the Sav1866 exporter. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 1977-1990.	2.6	59
31	A robust metallo-oxidase from the hyperthermophilic bacterium <i>Aquifex aeolicus</i> . <i>FEBS Journal</i> , 2007, 274, 2683-2694.	4.7	51
32	A Biochemical and Molecular Characterization of LEP1, an Extensin Peroxidase from Lupin. <i>Journal of Biological Chemistry</i> , 2003, 278, 41389-41399.	3.4	50
33	The <i>caa3</i> terminal oxidase of the thermohalophilic bacterium <i>Rhodothermus marinus</i> : a HiPIP:oxygen oxidoreductase lacking the key glutamate of the D-channel. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 1999, 1413, 1-13.	1.0	49
34	The tetraheme cytochrome from <i>Shewanella oneidensis</i> MR-1 shows thermodynamic bias for functional specificity of the hemes. <i>Journal of Biological Inorganic Chemistry</i> , 2009, 14, 375-385.	2.6	48
35	The multicopper oxidase from the archaeon <i>Pyrobaculum aerophilum</i> shows nitrous oxide reductase activity. <i>FEBS Journal</i> , 2010, 277, 3176-3189.	4.7	48
36	New targets for drug design: importance of nsp14/nsp10 complex formation for the 3'â€™â€™5'â€™â€™ exonucleolytic activity on SARS-CoV-2. <i>FEBS Journal</i> , 2021, 288, 5130-5147.	4.7	48

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37	Nine-haem cytochrome c from <i>Desulfovibrio desulfuricans</i> ATCC 27774: primary sequence determination, crystallographic refinement at 1.8 Å and modelling studies of its interaction with the tetrahaem cytochrome c 3. <i>Journal of Biological Inorganic Chemistry</i> , 1999, 4, 478-494.	2.6	46
38	Improvement of side-chain modeling in proteins with the self-consistent mean field theory method based on an analysis of the factors influencing prediction. , 1999, 50, 111-131.		44
39	Structural consequences of ATP hydrolysis on the ABC transporter NBD dimer: Molecular dynamics studies of HlyB. <i>Protein Science</i> , 2011, 20, 1220-1230.	7.6	43
40	Characterization of the periplasmic redox network that sustains the versatile anaerobic metabolism of <i>Shewanella oneidensis</i> MR-1. <i>Frontiers in Microbiology</i> , 2015, 6, 665.	3.5	42
41	Analyzing the Molecular Basis of Enzyme Stability in Ethanol/Water Mixtures Using Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 465-473.	5.4	41
42	A molecular perspective on nonaqueous biocatalysis: contributions from simulation studies. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13723.	2.8	41
43	The Mechanism of Superoxide Scavenging by <i>Archaeoglobus fulgidus</i> Neelaredoxin. <i>Journal of Biological Chemistry</i> , 2001, 276, 38995-39001.	3.4	39
44	Conformational Component in the Coupled Transfer of Multiple Electrons and Protons in a Monomeric Tetraheme Cytochrome. <i>Journal of Biological Chemistry</i> , 2001, 276, 44044-44051.	3.4	39
45	The lactate dehydrogenases encoded by the <i>ldhA</i> and <i>ldhB</i> genes in <i>Lactococcus lactis</i> exhibit distinct regulation and catalytic properties: comparative modeling to probe the molecular basis. <i>FEBS Journal</i> , 2007, 274, 5924-5936.	4.7	39
46	Cutinase Activity and Enantioselectivity in Supercritical Fluids. <i>Industrial & Engineering Chemistry Research</i> , 1998, 37, 3189-3194.	3.7	38
47	Role of the Anti-Sigma Factor SpoIIAB in Regulation of σ^G during <i>Bacillus subtilis</i> Sporulation. <i>Journal of Bacteriology</i> , 2004, 186, 4000-4013.	2.2	38
48	Water Dependent Properties of Cutinase in Nonaqueous Solvents: A Computational Study of Enantioselectivity. <i>Biophysical Journal</i> , 2005, 89, 999-1008.	0.5	38
49	The rice cold-responsive calcium-dependent protein kinase OsCPK17 is regulated by alternative splicing and post-translational modifications. <i>Biochimica Et Biophysica Acta - Molecular Cell Research</i> , 2018, 1865, 231-246.	4.1	38
50	Comparative redox and pK _a calculations on cytochrome c 3 from several <i>Desulfovibrio</i> species using continuum electrostatic methods. <i>Journal of Biological Inorganic Chemistry</i> , 1999, 4, 73-86.	2.6	37
51	Gene Cluster of <i>Rhodothermus marinus</i> High-Potential Iron-Sulfur Protein: Oxygen Oxidoreductase, a <i>caa 3</i> -Type Oxidase Belonging to the Superfamily of Heme-Copper Oxidases. <i>Journal of Bacteriology</i> , 2001, 183, 687-699.	2.2	35
52	Theoretical studies on the redox-Bohr effect in cytochrome c 3 from <i>Desulfovibrio vulgaris</i> Hildenborough. <i>Journal of Biological Inorganic Chemistry</i> , 1997, 2, 714-727.	2.6	33
53	An iterative structure-assisted approach to sequence alignment and comparative modeling. , 1999, 37, 55-60.		32
54	Unexplored Nucleotide Binding Modes for the ABC Exporter MsbA. <i>Journal of the American Chemical Society</i> , 2018, 140, 14112-14125.	13.7	32

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55	Effect of immobilization support, water activity, and enzyme ionization state on cutinase activity and enantioselectivity in organic media. <i>Biotechnology and Bioengineering</i> , 2004, 85, 442-449.	3.3	31
56	Insights into the Molecular Mechanism of an ABC Transporter: Conformational Changes in the NBD Dimer of MJ0796. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5486-5496.	2.6	31
57	Design of a Peptidic Turn with High Affinity for Hg ^{II} . <i>Inorganic Chemistry</i> , 2012, 51, 11339-11348.	4.0	31
58	Molecular Dynamics Simulation of Cytochrome c3: Studying the Reduction Processes Using Free Energy Calculations. <i>Biophysical Journal</i> , 1998, 74, 1708-1721.	0.5	30
59	Self-Assembly Molecular Dynamics Simulations Shed Light into the Interaction of the Influenza Fusion Peptide with a Membrane Bilayer. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 795-805.	5.4	30
60	Structure of Escherichia coli Flavodiiron Nitric Oxide Reductase. <i>Journal of Molecular Biology</i> , 2016, 428, 4686-4707.	4.2	30
61	The role of Asp116 in the reductive cleavage of dioxygen to water in CotA laccase: assistance during the proton-transfer mechanism. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 186-193.	2.5	29
62	Inter-domain Communication Mechanisms in an ABC Importer: A Molecular Dynamics Study of the MalFGK2E Complex. <i>PLoS Computational Biology</i> , 2011, 7, e1002128.	3.2	28
63	Predicting the Thermodynamics and Kinetics of Helix Formation in a Cyclic Peptide Model. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5148-5157.	5.3	28
64	Putative dioxygen-binding sites and recognition of tigecycline and minocycline in the tetracycline-degrading monooxygenase TetX. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 1758-1767.	2.5	28
65	An electrogenic redox loop in sulfate reduction reveals a likely widespread mechanism of energy conservation. <i>Nature Communications</i> , 2018, 9, 5448.	12.8	27
66	Incorporating knowledge-based biases into an energy-based side-chain modeling method: Application to comparative modeling of protein structure. <i>Biopolymers</i> , 2001, 59, 72-86.	2.4	26
67	CytochromecOxidase as a Calcium Binding Protein. Studies on the Role of a Conserved Aspartate in Helices XI [~] XII Cytoplasmic Loop in Cation Binding. <i>Biochemistry</i> , 2005, 44, 12391-12401.	2.5	26
68	Functional Domains of the Bacillus subtilis Transcription Factor AraR and Identification of Amino Acids Important for Nucleoprotein Complex Assembly and Effector Binding. <i>Journal of Bacteriology</i> , 2006, 188, 3024-3036.	2.2	26
69	Structural features of [NiFeSe] and [NiFe] hydrogenases determining their different properties: a computational approach. <i>Journal of Biological Inorganic Chemistry</i> , 2012, 17, 543-555.	2.6	26
70	Redox-Bohr and Other Cooperativity Effects in the Nine-heme Cytochrome c from <i>Desulfovibrio desulfuricans</i> ATCC 27774. <i>Journal of Biological Chemistry</i> , 2003, 278, 36455-36469.	3.4	25
71	Superoxide reduction by <i>Nanoarchaeum equitans</i> neelaredoxin, an enzyme lacking the highly conserved glutamate iron ligand. <i>Journal of Biological Inorganic Chemistry</i> , 2008, 13, 219-228.	2.6	24
72	On the stability and plastic properties of the interior L3 loop in <i>R.capsulatus</i> porin. A molecular dynamics study. <i>Protein Engineering, Design and Selection</i> , 1994, 7, 487-493.	2.1	23

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73	Modeling Electron Transfer Thermodynamics in Protein Complexes: Interaction between Two Cytochromes c3. <i>Biophysical Journal</i> , 2004, 86, 2773-2785.	0.5	23
74	Influence of the protein structure surrounding the active site on the catalytic activity of [NiFeSe] hydrogenases. <i>Journal of Biological Inorganic Chemistry</i> , 2013, 18, 419-427.	2.6	23
75	AOX1-Subfamily Gene Members in <i>Olea europaea</i> cv. "Galega Vulgaris" Gene Characterization and Expression of Transcripts during IBA-Induced in Vitro Adventitious Rooting. <i>International Journal of Molecular Sciences</i> , 2018, 19, 597.	4.1	23
76	Reorganization and Conformational Changes in the Reduction of Tetraheme Cytochromes. <i>Biophysical Journal</i> , 2005, 89, 3919-3930.	0.5	22
77	Exploring O ₂ Diffusion in A-Type Cytochrome c Oxidases: Molecular Dynamics Simulations Uncover Two Alternative Channels towards the Binuclear Site. <i>PLoS Computational Biology</i> , 2014, 10, e1004010.	3.2	22
78	Structural and Functional insights into the catalytic mechanism of the Type II NADH:quinone oxidoreductase family. <i>Scientific Reports</i> , 2017, 7, 42303.	3.3	22
79	Effects of protein-protein interactions on electron transfer: docking and electron transfer calculations for complexes between flavodoxin and c-type cytochromes. <i>Journal of Biological Inorganic Chemistry</i> , 1999, 4, 360-374.	2.6	21
80	Investigation of protonatable residues in <i>Rhodothermus marinus</i> cca 3 haem-copper oxygen reductase: comparison with <i>Paracoccus denitrificans</i> aa 3 haem-copper oxygen reductase. <i>Journal of Biological Inorganic Chemistry</i> , 2004, 9, 124-134.	2.6	21
81	Membrane-Induced Conformational Changes of Kyotorphin Revealed by Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11659-11667.	2.6	21
82	Structural and Functional Characterization of an Ancient Bacterial Transglutaminase Sheds Light on the Minimal Requirements for Protein Cross-Linking. <i>Biochemistry</i> , 2015, 54, 5723-5734.	2.5	21
83	Docking and electron transfer studies between rubredoxin and rubredoxin:oxygen oxidoreductase. <i>Journal of Biological Inorganic Chemistry</i> , 2003, 8, 475-488.	2.6	20
84	Molecular basis for redox-Bohr and cooperative effects in cytochrome c3 from <i>Desulfovibrio desulfuricans</i> ATCC 27774: Crystallographic and modeling studies of oxidized and reduced high-resolution structures at pH 7.6. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 54, 135-152.	2.6	20
85	Coupling between protonation and conformation in cytochrome c oxidase: Insights from constant-pH MD simulations. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2016, 1857, 759-771.	1.0	20
86	F508del disturbs the dynamics of the nucleotide binding domains of CFTR before and after ATP hydrolysis. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020, 88, 113-126.	2.6	20
87	Dioxygen and nitric oxide pathways and affinity to the catalytic site of rubredoxin:oxygen oxidoreductase from <i>Desulfovibrio gigas</i> . <i>Journal of Biological Inorganic Chemistry</i> , 2009, 14, 853-862.	2.6	18
88	The Role of Lys147 in the Interaction between MPSA-Gold Nanoparticles and the β -Hemolysin Nanopore. <i>Langmuir</i> , 2012, 28, 15643-15650.	3.5	18
89	Regulation of the mechanism of Type-II NADH: Quinone oxidoreductase from <i>S. aureus</i> . <i>Redox Biology</i> , 2018, 16, 209-214.	9.0	18
90	A LysM Domain Intervenes in Sequential Protein-Protein and Protein-Peptidoglycan Interactions Important for Spore Coat Assembly in <i>Bacillus subtilis</i> . <i>Journal of Bacteriology</i> , 2019, 201, .	2.2	18

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91	Conformational and Orientational Guidance of the Analgesic Dipeptide Kyotorphin Induced by Lipidic Membranes: Putative Correlation toward Receptor Docking. <i>Journal of Physical Chemistry B</i> , 2006, 110, 3385-3394.	2.6	17
92	The key role of glutamate 172 in the mechanism of type II NADH:quinone oxidoreductase of <i>Staphylococcus aureus</i> . <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2017, 1858, 823-832.	1.0	17
93	Implicit solvation in the self-consistent mean field theory method: sidechain modelling and prediction of folding free energies of protein mutants. <i>Journal of Computer-Aided Molecular Design</i> , 2001, 15, 721-740.	2.9	16
94	Probing key DNA contacts in AraR-mediated transcriptional repression of the <i>Bacillus subtilis</i> arabinose regulon. <i>Nucleic Acids Research</i> , 2007, 35, 4755-4766.	14.5	16
95	The Pathway for O ₂ Diffusion inside CotA Laccase and Possible Implications on the Multicopper Oxidases Family. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3525-3531.	5.3	15
96	Structural Analysis of <i>Thermus thermophilus</i> HB27 Mannosyl-3-phosphoglycerate Synthase Provides Evidence for a Second Catalytic Metal Ion and New Insight into the Retaining Mechanism of Glycosyltransferases. <i>Journal of Biological Chemistry</i> , 2010, 285, 17857-17868.	3.4	14
97	Simulation of multihaem cytochromes. <i>FEBS Letters</i> , 2012, 586, 510-518.	2.8	14
98	Effect of pH on the influenza fusion peptide properties unveiled by constant-pH molecular dynamics simulations combined with experiment. <i>Scientific Reports</i> , 2020, 10, 20082.	3.3	14
99	Structural determinants of ligand imprinting: A molecular dynamics simulation study of subtilisin in aqueous and apolar solvents. <i>Protein Science</i> , 2011, 20, 379-386.	7.6	13
100	Molecular modeling of hair keratin/peptide complex: Using MM-PBSA calculations to describe experimental binding results. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 1409-1417.	2.6	13
101	Natural Domain Design: Enhanced Thermal Stability of a Zinc-Lacking Ferredoxin Isoform Shows that a Hydrophobic Core Efficiently Replaces the Structural Metal Site. <i>Biochemistry</i> , 2006, 45, 10376-10384.	2.5	12
102	Study of the interactions of bovine serum albumin with a molybdenum(II) carbonyl complex by spectroscopic and molecular simulation methods. <i>PLoS ONE</i> , 2018, 13, e0204624.	2.5	12
103	Fusing simulation and experiment: The effect of mutations on the structure and activity of the influenza fusion peptide. <i>Scientific Reports</i> , 2016, 6, 28099.	3.3	10
104	Molecular structure of FoxE, the putative iron oxidase of <i>Rhodobacter ferrooxidans</i> SW2. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2017, 1858, 847-853.	1.0	10
105	Specific amino acids of Olive mild mosaic virus coat protein are involved in transmission by <i>Olpidium brassicae</i> . <i>Journal of General Virology</i> , 2011, 92, 2209-2213.	2.9	10
106	The nsp15 Nuclease as a Good Target to Combat SARS-CoV-2: Mechanism of Action and Its Inactivation with FDA-Approved Drugs. <i>Microorganisms</i> , 2022, 10, 342.	3.6	10
107	Ionic strength dependence of the non-physiological electron transfer between flavodoxin and cytochrome c 553 from <i>D. vulgaris</i> . <i>Journal of Biological Inorganic Chemistry</i> , 2000, 5, 730-737.	2.6	9
108	The Bsmoc group as a novel scaffold for the design of irreversible inhibitors of cysteine proteases. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2006, 16, 2738-2741.	2.2	9

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109	Structural Determinants for the Membrane Insertion of the Transmembrane Peptide of Hemagglutinin from Influenza Virus. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 3001-3012.	5.4	9
110	Insights into the structure of the diiron site of RIC from <i>Escherichia coli</i> . <i>FEBS Letters</i> , 2015, 589, 426-431.	2.8	9
111	Molecular mechanisms of the influenza fusion peptide: insights from experimental and simulation studies. <i>FEBS Open Bio</i> , 2021, 11, 3253-3261.	2.3	9
112	Theoretical Identification of Proton Channels in the Quinol Oxidase aa3 from <i>Acidianus ambivalens</i> . <i>Biophysical Journal</i> , 2004, 87, 4316-4325.	0.5	8
113	Interaction of Counterions with Subtilisin in Acetonitrile: Insights from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5838-5848.	2.6	7
114	Effect of a pH Gradient on the Protonation States of Cytochrome <i>c</i> Oxidase: A Continuum Electrostatics Study. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 256-266.	5.4	5
115	Studying O ₂ pathways in [NiFe]- and [NiFeSe]-hydrogenases. <i>Scientific Reports</i> , 2020, 10, 10540.	3.3	5
116	Molecular determinants for FMN binding in <i>Desulfovibrio gigas</i> flavodoxin. <i>FEBS Letters</i> , 2007, 581, 4397-4402.	2.8	4
117	The importance of the Abn2 calcium cluster in the endo-1,5-arabinanase activity from <i>Bacillus subtilis</i> . <i>Journal of Biological Inorganic Chemistry</i> , 2014, 19, 505-513.	2.6	4
118	Parainfluenza Fusion Peptide Promotes Membrane Fusion by Assembling into Oligomeric Porelike Structures. <i>ACS Chemical Biology</i> , 2022, 17, 1831-1843.	3.4	3
119	The Importance of Lipid Conjugation on Anti-Fusion Peptides against Nipah Virus. <i>Biomedicines</i> , 2022, 10, 703.	3.2	2
120	Protein thermal stabilization by charged compatible solutes: Computational studies in rubredoxin from <i>Desulfovibrio gigas</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 72, 580-588.	2.6	1
121	Understanding the Special Properties of [NiFeSe] Hydrogenases through the Use of Computational Methodologies. <i>Biophysical Journal</i> , 2014, 106, 38a.	0.5	1
122	Molecular Dynamics Simulations Suggest a Possible Role for NO in the Polyol Synthesis of Silver Nanostructures. <i>Journal of Physical Chemistry C</i> , 2020, 124, 24279-24288.	3.1	1
123	ATP hydrolysis and nucleotide exit enhance maltose translocation in the MalFCK2E importer. <i>Scientific Reports</i> , 2021, 11, 10591.	3.3	1
124	The Amino Acids Motif -32GSSYN36- in the Catalytic Domain of <i>E. coli</i> Flavorubredoxin NO Reductase Is Essential for Its Activity. <i>Catalysts</i> , 2021, 11, 926.	3.5	1
125	Proton transfer mechanisms in multi-copper oxidases: studies in CotA-laccase. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, s170-s171.	0.3	1
126	Cutinase activity and enantioselectivity in supercritical fluids. <i>Progress in Biotechnology</i> , 1998, , 483-486.	0.2	0

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127	Structural analysis of <i>Thermus thermophilus</i> HB27 mannosyl-3-phosphoglycerate synthase. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2010, 66, s142-s142.	0.3	0
128	Modeling the Structural Properties of the Transmembrane Peptide of Influenza Hemagglutinin in a Membrane Bilayer. <i>Biophysical Journal</i> , 2014, 106, 53a.	0.5	0
129	MD Simulations Reveal an Alternative Pathway for Dioxygen Diffusion in Aa3 Cytochrome C Oxidases. <i>Biophysical Journal</i> , 2014, 106, 369a.	0.5	0
130	Structural Properties of Membrane Inserted Fusion Peptide from Influenza Virus Analysed by Molecular Simulation. <i>Biophysical Journal</i> , 2014, 106, 53a.	0.5	0
131	Structure of FoxE, the <i>Rhodobacter ferrooxidans</i> SW2 putative iron oxidase. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, C1175-C1175.	0.1	0
132	Modeling hydration mechanisms of enzymes in nonpolar and polar organic solvents. <i>FEBS Journal</i> , 2007, .	4.7	0