

Claudio M. Soares

List of Publications by Year in descending order

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132
papers

5,780
citations

81900
39
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88630
70
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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 1.8Å... 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. PLoS Pathogens, 2021, 17, e1009772.	4.7	74
20	Modeling hydration mechanisms of enzymes in nonpolar and polar organic solvents. FEBS Journal, 2007, 274, 2424-2436.	4.7	73
21	Mechanisms underlying dioxygen reduction in laccases. Structural and modelling studies focusing on proton transfer. BMC Structural Biology, 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. Biochimica Et Biophysica Acta - General Subjects, 2008, 1780, 905-913.	2.4	68
24	Pathways of H ₂ toward the Active Site of [NiFe]-Hydrogenase. Biophysical Journal, 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. Biochemical Journal, 2008, 412, 339-346.	3.7	66
26	Exploring the molecular mechanisms of electron shuttling across the microbe/metal space. Frontiers in Microbiology, 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. Biophysical Journal, 2005, 88, 4188-4199.	0.5	63
28	Proton pathways in a [NiFe]-hydrogenase: A theoretical study. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1010-1022.	2.6	63
29	Studies of the reduction and protonation behavior of tetraheme cytochromes using atomic detail. Journal of Biological Inorganic Chemistry, 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. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1977-1990.	2.6	59
31	A robust metallo-oxidase from the hyperthermophilic bacterium Aquifex aeolicus. FEBS Journal, 2007, 274, 2683-2694.	4.7	51
32	A Biochemical and Molecular Characterization of LEP1, an Extensin Peroxidase from Lupin. Journal of Biological Chemistry, 2003, 278, 41389-41399.	3.4	50
33	The caa3 terminal oxidase of the thermohalophilic bacterium Rhodothermus marinus: a HiPIP:oxygen oxidoreductase lacking the key glutamate of the D-channel. Biochimica Et Biophysica Acta - Bioenergetics, 1999, 1413, 1-13.	1.0	49
34	The tetraheme cytochrome from Shewanella oneidensis MR-1 shows thermodynamic bias for functional specificity of the hemes. Journal of Biological Inorganic Chemistry, 2009, 14, 375-385.	2.6	48
35	The multicopper oxidase from the archaeon <i>Pyrobaculum aerophilum</i> shows nitrous oxide reductase activity. FEBS Journal, 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€™ exoribonucleolytic activity on SARS-CoV-2. FEBS Journal, 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>ldh</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</i> 3-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	Cytochrome c Oxidase as a Calcium Binding Protein. Studies on the Role of a Conserved Aspartate in Helices XI and 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 Desulfovibrio desulfuricans ATCC 27774. <i>Journal of Biological Chemistry</i> , 2003, 278, 36455-36469.	3.4	25
71	Superoxide reduction by Nanoarchaeum equitans 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 R.capsulatus 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 O2 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> caa 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