Claudio M. Soares

List of Publications by Year
in descending order

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132 papers	5,780 citations	93792 39 h-index	100535 70 g-index
142 all docs	142 docs citations	142 times ranked	7162 citing authors

#	Article	IF	Citations
1	The nsp15 Nuclease as a Good Target to Combat SARS-CoV-2: Mechanism of Action and Its Inactivation with FDA-Approved Drugs. Microorganisms, 2022, 10, 342.	1.6	10
2	The Importance of Lipid Conjugation on Anti-Fusion Peptides against Nipah Virus. Biomedicines, 2022, 10, 703.	1.4	2
3	Parainfluenza Fusion Peptide Promotes Membrane Fusion by Assembling into Oligomeric Porelike Structures. ACS Chemical Biology, 2022, 17, 1831-1843.	1.6	3
4	New targets for drug design: importance of nsp14/nsp10 complex formation for the 3â€™â€5â€™ exoribonucleolytic activity on SARSâ€CoVâ€2. FEBS Journal, 2021, 288, 5130-5147.	2.2	48
5	ATP hydrolysis and nucleotide exit enhance maltose translocation in the MalFGK2E importer. Scientific Reports, 2021, 11, 10591.	1.6	1
6	The Amino Acids Motif -32GSSYN36- in the Catalytic Domain of E. coli Flavorubredoxin NO Reductase Is Essential for Its Activity. Catalysts, 2021, 11, 926.	1.6	1
7	Signatures in SARS-CoV-2 spike protein conferring escape to neutralizing antibodies. PLoS Pathogens, 2021, 17, e1009772.	2.1	74
8	Molecular mechanisms of the influenza fusion peptide: insights from experimental and simulation studies. FEBS Open Bio, 2021, 11, 3253-3261.	1.0	9
9	F508del disturbs the dynamics of the nucleotide binding domains of CFTR before and after ATP hydrolysis. Proteins: Structure, Function and Bioinformatics, 2020, 88, 113-126.	1.5	20
10	Molecular Dynamics Simulations Suggest a Possible Role for NO in the Polyol Synthesis of Silver Nanostructures. Journal of Physical Chemistry C, 2020, 124, 24279-24288.	1.5	1
11	Effect of pH on the influenza fusion peptide properties unveiled by constant-pH molecular dynamics simulations combined with experiment. Scientific Reports, 2020, 10, 20082.	1.6	14
12	Studying O2 pathways in [NiFe]- and [NiFeSe]-hydrogenases. Scientific Reports, 2020, 10, 10540.	1.6	5
13	A LysM Domain Intervenes in Sequential Protein-Protein and Protein-Peptidoglycan Interactions Important for Spore Coat Assembly in Bacillus subtilis. Journal of Bacteriology, 2019, 201, .	1.0	18
14	Regulation of the mechanism of Type-II NADH: Quinone oxidoreductase from S. aureus. Redox Biology, 2018, 16, 209-214.	3.9	18
15	The rice cold-responsive calcium-dependent protein kinase OsCPK17 is regulated by alternative splicing and post-translational modifications. Biochimica Et Biophysica Acta - Molecular Cell Research, 2018, 1865, 231-246.	1.9	38
16	An electrogenic redox loop in sulfate reduction reveals a likely widespread mechanism of energy conservation. Nature Communications, 2018, 9, 5448.	5.8	27
17	Unexplored Nucleotide Binding Modes for the ABC Exporter MsbA. Journal of the American Chemical Society, 2018, 140, 14112-14125.	6.6	32
18	Study of the interactions of bovine serum albumin with a molybdenum(II) carbonyl complex by spectroscopic and molecular simulation methods. PLoS ONE, 2018, 13, e0204624.	1.1	12

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19	AOX1-Subfamily Gene Members in Olea europaea cv. â€œGalega Vulgarâ€â€”Gene Characterization and Expression of Transcripts during IBA-Induced in Vitro Adventitious Rooting. International Journal of Molecular Sciences, 2018, 19, 597.	1.8	23
20	Effect of a pH Gradient on the Protonation States of Cytochrome c Oxidase: A Continuum Electrostatics Study. Journal of Chemical Information and Modeling, 2017, 57, 256-266.	2.5	5
21	Structural and Functional insights into the catalytic mechanism of the Type II NADH:quinone oxidoreductase family. Scientific Reports, 2017, 7, 42303.	1.6	22
22	Molecular structure of FoxE, the putative iron oxidase of Rhodobacter ferrooxidans SW2. Biochimica Et Biophysica Acta - Bioenergetics, 2017, 1858, 847-853.	0.5	10
23	The key role of glutamate 172 in the mechanism of type II NADH:quinone oxidoreductase of Staphylococcus aureus. Biochimica Et Biophysica Acta - Bioenergetics, 2017, 1858, 823-832.	0.5	17
24	Structure of FoxE, the Rhodobacter ferrooxidans SW2 putative iron oxidase. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1175-C1175.	0.0	0
25	Structure of Escherichia coli Flavodiiron Nitric Oxide Reductase. Journal of Molecular Biology, 2016, 428, 4686-4707.	2.0	30
26	Fusing simulation and experiment: The effect of mutations on the structure and activity of the influenza fusion peptide. Scientific Reports, 2016, 6, 28099.	1.6	10
27	Coupling between protonation and conformation in cytochrome c oxidase: Insights from constant-pH MD simulations. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 759-771.	0.5	20
28	Characterization of the periplasmic redox network that sustains the versatile anaerobic metabolism of Shewanella oneidensis MR-1. Frontiers in Microbiology, 2015, 6, 665.	1.5	42
29	Insights into the structure of the diiron site of RIC from Escherichia coli. FEBS Letters, 2015, 589, 426-431.	1.3	9
30	Self-Assembly Molecular Dynamics Simulations Shed Light into the Interaction of the Influenza Fusion Peptide with a Membrane Bilayer. Journal of Chemical Information and Modeling, 2015, 55, 795-805.	2.5	30
31	Structural and Functional Characterization of an Ancient Bacterial Transglutaminase Sheds Light on the Minimal Requirements for Protein Cross-Linking. Biochemistry, 2015, 54, 5723-5734.	1.2	21
32	Exploring O2 Diffusion in A-Type Cytochrome c Oxidases: Molecular Dynamics Simulations Uncover Two Alternative Channels towards the Binuclear Site. PLoS Computational Biology, 2014, 10, e1004010.	1.5	22
33	Exploring the molecular mechanisms of electron shuttling across the microbe/metal space. Frontiers in Microbiology, 2014, 5, 318.	1.5	65
34	Understanding the Special Properties of [NiFeSe] Hydrogenases through the Use of Computational Methodologies. Biophysical Journal, 2014, 106, 38a.	0.2	1
35	The importance of the Abn2 calcium cluster in the endo-1,5-arabinanase activity from Bacillus subtilis. Journal of Biological Inorganic Chemistry, 2014, 19, 505-513.	1.1	4
36	Modeling the Structural Properties of the Transmembrane Peptide of Influenza Hemagglutinin in a Membrane Bilayer. Biophysical Journal, 2014, 106, 53a.	0.2	0

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37	MD Simulations Reveal an Alternative Pathway for Dioxygen Diffusion in Aa3 Cytochrome C Oxidases. Biophysical Journal, 2014, 106, 369a.	0.2	0
38	The Pathway for O₂ Diffusion inside CotA Laccase and Possible Implications on the Multicopper Oxidases Family. Journal of Chemical Theory and Computation, 2014, 10, 3525-3531.	2.3	15
39	Structural Properties of Membrane Inserted Fusion Peptide from Influenza Virus Analysed by Molecular Simulation. Biophysical Journal, 2014, 106, 53a.	0.2	0
40	A molecular perspective on nonaqueous biocatalysis: contributions from simulation studies. Physical Chemistry Chemical Physics, 2013, 15, 13723.	1.3	41
41	Influence of the protein structure surrounding the active site on the catalytic activity of [NiFeSe] hydrogenases. Journal of Biological Inorganic Chemistry, 2013, 18, 419-427.	1.1	23
42	Predicting the Thermodynamics and Kinetics of Helix Formation in a Cyclic Peptide Model. Journal of Chemical Theory and Computation, 2013, 9, 5148-5157.	2.3	28
43	Mind the gap: cytochrome interactions reveal electron pathways across the periplasm of Shewanella oneidensis MR-1. Biochemical Journal, 2013, 449, 101-108.	1.7	129
44	Putative dioxygen-binding sites and recognition of tigecycline and minocycline in the tetracycline-degrading monooxygenase TetX. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 1758-1767.	2.5	28
45	Structural Determinants for the Membrane Insertion of the Transmembrane Peptide of Hemagglutinin from Influenza Virus. Journal of Chemical Information and Modeling, 2012, 52, 3001-3012.	2.5	9
46	Interaction of Counterions with Subtilisin in Acetonitrile: Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 5838-5848.	1.2	7
47	The Role of Lys147 in the Interaction between MPSA-Gold Nanoparticles and the Î±-Hemolysin Nanopore. Langmuir, 2012, 28, 15643-15650.	1.6	18
48	Design of a Peptidic Turn with High Affinity for Hg^{II}. Inorganic Chemistry, 2012, 51, 11339-11348.	1.9	31
49	Analyzing the Molecular Basis of Enzyme Stability in Ethanol/Water Mixtures Using Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2012, 52, 465-473.	2.5	41
50	The role of Asp116 in the reductive cleavage of dioxygen to water in CotA laccase: assistance during the proton-transfer mechanism. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 186-193.	2.5	29
51	Molecular modeling of hair keratin/peptide complex: Using MMâ€PBSA calculations to describe experimental binding results. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1409-1417.	1.5	13
52	Structural features of [NiFeSe] and [NiFe] hydrogenases determining their different properties: a computational approach. Journal of Biological Inorganic Chemistry, 2012, 17, 543-555.	1.1	26
53	Simulation of multihaem cytochromes. FEBS Letters, 2012, 586, 510-518.	1.3	14
54	Conformational changes induced by ATPâ€hydrolysis in an ABC transporter: A molecular dynamics study of the Sav1866 exporter. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1977-1990.	1.5	59

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55	Structural determinants of ligand imprinting: A molecular dynamics simulation study of subtilisin in aqueous and apolar solvents. Protein Science, 2011, 20, 379-386.	3.1	13
56	Structural consequences of ATP hydrolysis on the ABC transporter NBD dimer: Molecular dynamics studies of HlyB. Protein Science, 2011, 20, 1220-1230.	3.1	43
57	Nickelâ€“Ironâ€“Selenium Hydrogenases â€“ An Overview. European Journal of Inorganic Chemistry, 2011, 2011, 948-962.	1.0	86
58	Inter-domain Communication Mechanisms in an ABC Importer: A Molecular Dynamics Study of the MalFGK2E Complex. PLoS Computational Biology, 2011, 7, e1002128.	1.5	28
59	Specific amino acids of Olive mild mosaic virus coat protein are involved in transmission by Olpidium brassicae. Journal of General Virology, 2011, 92, 2209-2213.	1.3	10
60	Structural analysis ofThermus thermophilusHB27 mannosyl-3-phosphoglycerate synthase. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, s142-s142.	0.3	0
61	Mechanisms underlying dioxygen reduction in laccases. Structural and modelling studies focusing on proton transfer. BMC Structural Biology, 2010, 10, 28.	2.3	72
62	The multicopper oxidase from the archaeon Pyrobaculumâ€ƒaerophilum shows nitrous oxide reductase activity. FEBS Journal, 2010, 277, 3176-3189.	2.2	48
63	Structural Analysis of Thermus thermophilus HB27 Mannosyl-3-phosphoglycerate Synthase Provides Evidence for a Second Catalytic Metal Ion and New Insight into the Retaining Mechanism of Glycosyltransferases. Journal of Biological Chemistry, 2010, 285, 17857-17868.	1.6	14
64	Membrane-Induced Conformational Changes of Kyotorphin Revealed by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 11659-11667.	1.2	21
65	Insights into the Molecular Mechanism of an ABC Transporter: Conformational Changes in the NBD Dimer of MJ0796. Journal of Physical Chemistry B, 2010, 114, 5486-5496.	1.2	31
66	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.	1.1	48
67	Dioxygen and nitric oxide pathways and affinity to the catalytic site of rubredoxin:oxygen oxidoreductase from Desulfovibrio gigas. Journal of Biological Inorganic Chemistry, 2009, 14, 853-862.	1.1	18
68	Proton transfer mechanisms in multi-copper oxidases: studies in CotA-laccase. Acta Crystallographica Section A: Foundations and Advances, 2009, 65, s170-s171.	0.3	1
69	Superoxide reduction by Nanoarchaeum equitans neelaredoxin, an enzyme lacking the highly conserved glutamate iron ligand. Journal of Biological Inorganic Chemistry, 2008, 13, 219-228.	1.1	24
70	Proton pathways in a [NiFe]â€hydrogenase: A theoretical study. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1010-1022.	1.5	63
71	Protein thermal stabilization by charged compatible solutes: Computational studies in rubredoxin from Desulfovibrio gigas. Proteins: Structure, Function and Bioinformatics, 2008, 72, 580-588.	1.5	1
72	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.	1.1	68

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73	Protein Structure and Dynamics in Ionic Liquids. Insights from Molecular Dynamics Simulation Studies. Journal of Physical Chemistry B, 2008, 112, 2566-2572.	1.2	199
74	Proximal mutations at the typeÂ1 copper site of CotA laccase: spectroscopic, redox, kinetic and structural characterization of I494A and L386A mutants. Biochemical Journal, 2008, 412, 339-346.	1.7	66
75	Probing key DNA contacts in AraR-mediated transcriptional repression of the Bacillus subtilis arabinose regulon. Nucleic Acids Research, 2007, 35, 4755-4766.	6.5	16
76	Molecular determinants for FMNâ€binding in Desulfovibrio gigas flavoredoxin. FEBS Letters, 2007, 581, 4397-4402.	1.3	4
77	Tailoring cutinase activity towards polyethylene terephthalate and polyamide 6,6 fibers. Journal of Biotechnology, 2007, 128, 849-857.	1.9	161
78	Modeling hydration mechanisms of enzymes in nonpolar and polar organic solvents. FEBS Journal, 2007, 274, 2424-2436.	2.2	73
79	A robust metallo-oxidase from the hyperthermophilic bacterium Aquifex aeolicus. FEBS Journal, 2007, 274, 2683-2694.	2.2	51
80	The lactate dehydrogenases encoded by the ldh and ldhB genes in Lactococcus lactis exhibit distinct regulation and catalytic propertiesâ€ƒâ€”comparative modeling to probe the molecular basis. FEBS Journal, 2007, 274, 5924-5936.	2.2	39
81	Modeling hydration mechanisms of enzymes in nonpolar and polar organic solvents. FEBS Journal, 2007, .	2.2	0
82	Conformational and Orientational Guidance of the Analgesic Dipeptide Kyotorphin Induced by Lipidic Membranes:â€‰ Putative Correlation toward Receptor Docking. Journal of Physical Chemistry B, 2006, 110, 3385-3394.	1.2	17
83	Pathways of H2 toward the Active Site of [NiFe]-Hydrogenase. Biophysical Journal, 2006, 91, 2035-2045.	0.2	66
84	Parametrization of 1-Butyl-3-methylimidazolium Hexafluorophosphate/Nitrate Ionic Liquid for the GROMOS Force Field. Journal of Physical Chemistry B, 2006, 110, 14444-14451.	1.2	131
85	Natural Domain Design:Â Enhanced Thermal Stability of a Zinc-Lacking Ferredoxin Isoform Shows that a Hydrophobic Core Efficiently Replaces the Structural Metal Siteâ€. Biochemistry, 2006, 45, 10376-10384.	1.2	12
86	The Bsmoc group as a novel scaffold for the design of irreversible inhibitors of cysteine proteases. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 2738-2741.	1.0	9
87	Revertant mutants G550E and 4RK rescue cystic fibrosis mutants in the first nucleotide-binding domain of CFTR by different mechanisms. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 17891-17896.	3.3	112
88	Functional Domains of the Bacillus subtilis Transcription Factor AraR and Identification of Amino Acids Important for Nucleoprotein Complex Assembly and Effector Binding. Journal of Bacteriology, 2006, 188, 3024-3036.	1.0	26
89	Sulphate respiration from hydrogen in Desulfovibrio bacteria: a structural biology overview. Progress in Biophysics and Molecular Biology, 2005, 89, 292-329.	1.4	141
90	Hydrogenases in Desulfovibrio vulgaris Hildenborough: structural and physiologic characterisation of the membrane-bound [NiFeSe] hydrogenase. Journal of Biological Inorganic Chemistry, 2005, 10, 667-682.	1.1	83

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91	Electric-Field-Induced Redox Potential Shifts of Tetraheme Cytochromes c3 Immobilized on Self-Assembled Monolayers: Surface-Enhanced Resonance Raman Spectroscopy and Simulation Studies. Biophysical Journal, 2005, 88, 4188-4199.	0.2	63
92	On the Use of Different Dielectric Constants for Computing Individual and Pairwise Terms in Poissonâ^'Boltzmann Studies of Protein Ionization Equilibrium. Journal of Physical Chemistry B, 2005, 109, 14691-14706.	1.2	91
93	Water Dependent Properties of Cutinase in Nonaqueous Solvents: A Computational Study of Enantioselectivity. Biophysical Journal, 2005, 89, 999-1008.	0.2	38
94	Reorganization and Conformational Changes in the Reduction of Tetraheme Cytochromes. Biophysical Journal, 2005, 89, 3919-3930.	0.2	22
95	CytochromecOxidase as a Calcium Binding Protein. Studies on the Role of a Conserved Aspartate in Helices XIâ^'XII Cytoplasmic Loop in Cation Bindingâ€. Biochemistry, 2005, 44, 12391-12401.	1.2	26
96	Role of the Anti-Sigma Factor SpoIIAB in Regulation of ÏƒG during Bacillus subtilis Sporulation. Journal of Bacteriology, 2004, 186, 4000-4013.	1.0	38
97	Investigation of protonatable residues in Rhodothermus marinus caa 3 haem-copper oxygen reductase: comparison with Paracoccus denitrificans aa 3 haem-copper oxygen reductase. Journal of Biological Inorganic Chemistry, 2004, 9, 124-134.	1.1	21
98	Effect of immobilization support, water activity, and enzyme ionization state on cutinase activity and enantioselectivity in organic media. Biotechnology and Bioengineering, 2004, 85, 442-449.	1.7	31
99	Theoretical Identification of Proton Channels in the Quinol Oxidase aa3 from Acidianus ambivalens. Biophysical Journal, 2004, 87, 4316-4325.	0.2	8
100	Modeling Electron Transfer Thermodynamics in Protein Complexes: Interaction between Two Cytochromes c3. Biophysical Journal, 2004, 86, 2773-2785.	0.2	23
101	Docking and electron transfer studies between rubredoxin and rubredoxin:oxygen oxidoreductase. Journal of Biological Inorganic Chemistry, 2003, 8, 475-488.	1.1	20
102	Molecular basis for redox-Bohr and cooperative effects in cytochrome c3 from Desulfovibrio desulfuricans ATCC 27774: Crystallographic and modeling studies of oxidized and reduced high-resolution structures at pH 7.6. Proteins: Structure, Function and Bioinformatics, 2003, 54, 135-152.	1.5	20
103	Protein Structure and Dynamics in Nonaqueous Solvents: Insights from Molecular Dynamics Simulation Studies. Biophysical Journal, 2003, 84, 1628-1641.	0.2	110
104	Redox-Bohr and Other Cooperativity Effects in the Nine-heme Cytochrome c from Desulfovibrio desulfuricans ATCC 27774. Journal of Biological Chemistry, 2003, 278, 36455-36469.	1.6	25
105	A Biochemical and Molecular Characterization of LEP1, an Extensin Peroxidase from Lupin. Journal of Biological Chemistry, 2003, 278, 41389-41399.	1.6	50
106	Constant-pH molecular dynamics using stochastic titration. Journal of Chemical Physics, 2002, 117, 4184-4200.	1.2	283
107	Molecular and Biochemical Characterization of a Highly Stable Bacterial Laccase That Occurs as a Structural Component of the Bacillus subtilis Endospore Coat. Journal of Biological Chemistry, 2002, 277, 18849-18859.	1.6	456
108	Studies of the reduction and protonation behavior of tetraheme cytochromes using atomic detail. Journal of Biological Inorganic Chemistry, 2002, 7, 200-216.	1.1	61

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109	Some Theoretical and Computational Aspects of the Inclusion of Proton Isomerism in the Protonation Equilibrium of Proteins. Journal of Physical Chemistry B, 2001, 105, 293-309.	1.2	122
110	[NiFe] hydrogenase from Desulfovibrio desulfuricans ATCC 27774: gene sequencing, three-dimensional structure determination and refinement at 1.8ÂÃ... and modelling studies of its interaction with the tetrahaem cytochrome c 3. Journal of Biological Inorganic Chemistry, 2001, 6, 63-81.	1.1	198
111	Incorporating knowledge-based biases into an energy-based side-chain modeling method: Application to comparative modeling of protein structure. Biopolymers, 2001, 59, 72-86.	1.2	26
112	Implicit solvation in the self-consistent mean field theory method: sidechain modelling and prediction of folding free energies of protein mutants. Journal of Computer-Aided Molecular Design, 2001, 15, 721-740.	1.3	16
113	The Mechanism of Superoxide Scavenging byArchaeoglobus fulgidus Neelaredoxin. Journal of Biological Chemistry, 2001, 276, 38995-39001.	1.6	39
114	Conformational Component in the Coupled Transfer of Multiple Electrons and Protons in a Monomeric Tetraheme Cytochrome. Journal of Biological Chemistry, 2001, 276, 44044-44051.	1.6	39
115	Gene Cluster of Rhodothermus marinus High-Potential Iron-Sulfur Protein:Oxygen Oxidoreductase, a caa 3 -Type Oxidase Belonging to the Superfamily of Heme-Copper Oxidases. Journal of Bacteriology, 2001, 183, 687-699.	1.0	35
116	Evolution of the Thyroid Hormone-Binding Protein, Transthyretin. General and Comparative Endocrinology, 2000, 119, 241-255.	0.8	182
117	Ionic strength dependence of the non-physiological electron transfer between flavodoxin and cytochrome c 553 from D. vulgaris. Journal of Biological Inorganic Chemistry, 2000, 5, 730-737.	1.1	9
118	Crystal Structure of Cardosin A, a Glycosylated and Arg-Gly-Asp-containing Aspartic Proteinase from the Flowers ofCynara cardunculus L.. Journal of Biological Chemistry, 1999, 274, 27694-27701.	1.6	82
119	Comparative redox and pK a calculations on cytochrome c 3 from several Desulfovibrio species using continuum electrostatic methods. Journal of Biological Inorganic Chemistry, 1999, 4, 73-86.	1.1	37
120	Effects of protein-protein interactions on electron transfer: docking and electron transfer calculations for complexes between flavodoxin and c-type cytochromes. Journal of Biological Inorganic Chemistry, 1999, 4, 360-374.	1.1	21
121	Nine-haem cytochrome c from Desulfovibrio desulfuricans ATCC 27774â€Š:â€Šprimary sequence determination, crystallographic refinement at 1.8â€‰ and modelling studies of its interaction with the tetrahaem cytochrome c 3. Journal of Biological Inorganic Chemistry, 1999, 4, 478-494.	1.1	46
122	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
123	An iterative structure-assisted approach to sequence alignment and comparative modeling. , 1999, 37, 55-60.		32
124	Improved modeling of side-chains in proteins with rotamer-based methods: A flexible rotamer model. , 1999, 37, 530-543.		68
125	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.	0.5	49
126	Simulation of Electron-Proton Coupling with a Monte Carlo Method: Application to Cytochrome c3 Using Continuum Electrostatics. Biophysical Journal, 1999, 76, 2978-2998.	0.2	105

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127	Cutinase Activity and Enantioselectivity in Supercritical Fluids. Industrial & Engineering Chemistry Research, 1998, 37, 3189-3194.	1.8	38
128	Molecular Dynamics Simulation of Cytochrome c3: Studying the Reduction Processes Using Free Energy Calculations. Biophysical Journal, 1998, 74, 1708-1721.	0.2	30
129	Cutinase activity and enantioselectivity in supercritical fluids. Progress in Biotechnology, 1998, , 483-486.	0.2	0
130	Theoretical studies on the redox-Bohr effect in cytochrome c 3 from Desulfovibrio vulgaris Hildenborough. Journal of Biological Inorganic Chemistry, 1997, 2, 714-727.	1.1	33
131	Ab initio determination of the crystal structure of cytochrome c6 and comparison with plastocyanin. Structure, 1995, 3, 1159-1169.	1.6	146
132	On the stability and plastic properties of the interior L3 loop in R.capsulatus porin. A molecular dynamics study. Protein Engineering, Design and Selection, 1994, 7, 487-493.	1.0	23