

Claudio M Soares

List of Publications by Year in descending order

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74
papers

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126708

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76
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76
times ranked

4118
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.	1.6	456
2	Constant-pH molecular dynamics using stochastic titration. <i>Journal of Chemical Physics</i> , 2002, 117, 4184-4200.	1.2	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.	1.2	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.	1.1	198
5	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.	1.4	141
6	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.	1.2	131
7	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.	1.2	122
8	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.	3.3	112
9	Protein Structure and Dynamics in Nonaqueous Solvents: Insights from Molecular Dynamics Simulation Studies. <i>Biophysical Journal</i> , 2003, 84, 1628-1641.	0.2	110
10	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.	0.2	105
11	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.	1.2	91
12	Nickel-Iron-Selenium Hydrogenases – An Overview. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 948-962.	1.0	86
13	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.	1.1	83
14	Modeling hydration mechanisms of enzymes in nonpolar and polar organic solvents. <i>FEBS Journal</i> , 2007, 274, 2424-2436.	2.2	73
15	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
16	Improved modeling of side-chains in proteins with rotamer-based methods: A flexible rotamer model. , 1999, 37, 530-543.		68
17	Pathways of H ₂ toward the Active Site of [NiFe]-Hydrogenase. <i>Biophysical Journal</i> , 2006, 91, 2035-2045.	0.2	66
18	Proximal mutations at the type 1 copper site of CotA laccase: spectroscopic, redox, kinetic and structural characterization of I494A and L386A mutants. <i>Biochemical Journal</i> , 2008, 412, 339-346.	1.7	66

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19	Electric-Field-Induced Redox Potential Shifts of Tetraheme Cytochromes c3 Immobilized on Self-Assembled Monolayers: Surface-Enhanced Resonance Raman Spectroscopy and Simulation Studies. <i>Biophysical Journal</i> , 2005, 88, 4188-4199.	0.2	63
20	Proton pathways in a [NiFe]â€hydrogenase: A theoretical study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 1010-1022.	1.5	63
21	Studies of the reduction and protonation behavior of tetraheme cytochromes using atomic detail. <i>Journal of Biological Inorganic Chemistry</i> , 2002, 7, 200-216.	1.1	61
22	Conformational changes induced by ATPâ€hydrolysis in an ABC transporter: A molecular dynamics study of the Sav1866 exporter. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 1977-1990.	1.5	59
23	A robust metallo-oxidase from the hyperthermophilic bacterium <i>Aquifex aeolicus</i> . <i>FEBS Journal</i> , 2007, 274, 2683-2694.	2.2	51
24	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.	1.1	48
25	The multicopper oxidase from the archaeon <i>Pyrobaculum aerophilum</i> shows nitrous oxide reductase activity. <i>FEBS Journal</i> , 2010, 277, 3176-3189.	2.2	48
26	Nine-haem cytochrome c from <i>Desulfovibrio desulfuricans</i> ATCC 27774â€™s primary sequence determination, crystallographic refinement at 1.8â€™ and modelling studies of its interaction with the tetrahaem cytochrome c 3. <i>Journal of Biological Inorganic Chemistry</i> , 1999, 4, 478-494.	1.1	46
27	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
28	Structural consequences of ATP hydrolysis on the ABC transporter NBD dimer: Molecular dynamics studies of HlyB. <i>Protein Science</i> , 2011, 20, 1220-1230.	3.1	43
29	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.	2.5	41
30	A molecular perspective on nonaqueous biocatalysis: contributions from simulation studies. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13723.	1.3	41
31	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.	1.6	39
32	The lactate dehydrogenases encoded by the <i>ldh</i> and <i>ldhB</i> genes in <i>Lactococcus lactis</i> exhibit distinct regulation and catalytic propertiesâ€™ comparative modeling to probe the molecular basis. <i>FEBS Journal</i> , 2007, 274, 5924-5936.	2.2	39
33	Cutinase Activity and Enantioselectivity in Supercritical Fluids. <i>Industrial & Engineering Chemistry Research</i> , 1998, 37, 3189-3194.	1.8	38
34	Water Dependent Properties of Cutinase in Nonaqueous Solvents: A Computational Study of Enantioselectivity. <i>Biophysical Journal</i> , 2005, 89, 999-1008.	0.2	38
35	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.	1.1	37
36	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.	1.1	33

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37	An iterative structure-assisted approach to sequence alignment and comparative modeling. , 1999, 37, 55-60.		32
38	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.	1.7	31
39	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.	1.2	31
40	Structure of Escherichia coli Flavodiiron Nitric Oxide Reductase. <i>Journal of Molecular Biology</i> , 2016, 428, 4686-4707.	2.0	30
41	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
42	Inter-domain Communication Mechanisms in an ABC Importer: A Molecular Dynamics Study of the MalFGK2E Complex. <i>PLoS Computational Biology</i> , 2011, 7, e1002128.	1.5	28
43	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.	1.2	26
44	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.	1.1	26
45	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.	1.6	25
46	Modeling Electron Transfer Thermodynamics in Protein Complexes: Interaction between Two Cytochromes c3. <i>Biophysical Journal</i> , 2004, 86, 2773-2785.	0.2	23
47	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.	1.1	23
48	Reorganization and Conformational Changes in the Reduction of Tetraheme Cytochromes. <i>Biophysical Journal</i> , 2005, 89, 3919-3930.	0.2	22
49	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.	1.5	22
50	Structural and Functional insights into the catalytic mechanism of the Type II NADH:quinone oxidoreductase family. <i>Scientific Reports</i> , 2017, 7, 42303.	1.6	22
51	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.	1.1	21
52	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.	1.1	21
53	Membrane-Induced Conformational Changes of Kyotorphin Revealed by Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11659-11667.	1.2	21
54	Docking and electron transfer studies between rubredoxin and rubredoxin:oxygen oxidoreductase. <i>Journal of Biological Inorganic Chemistry</i> , 2003, 8, 475-488.	1.1	20

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55	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.	1.5	20
56	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.	0.5	20
57	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.	1.5	20
58	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.	1.1	18
59	The Role of Lys147 in the Interaction between MPSA-Gold Nanoparticles and the $\hat{\pm}$ -Hemolysin Nanopore. <i>Langmuir</i> , 2012, 28, 15643-15650.	1.6	18
60	Regulation of the mechanism of Type-II NADH: Quinone oxidoreductase from <i>S. aureus</i> . <i>Redox Biology</i> , 2018, 16, 209-214.	3.9	18
61	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, .	1.0	18
62	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.	0.5	17
63	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.	1.3	16
64	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.	2.3	15
65	Simulation of multihaem cytochromes. <i>FEBS Letters</i> , 2012, 586, 510-518.	1.3	14
66	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.	1.6	14
67	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.	3.1	13
68	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.	1.2	12
69	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.	1.1	12
70	Interaction of Counterions with Subtilisin in Acetonitrile: Insights from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5838-5848.	1.2	7
71	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.	2.5	5
72	Studying O ₂ pathways in [NiFe]- and [NiFeSe]-hydrogenases. <i>Scientific Reports</i> , 2020, 10, 10540.	1.6	5

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73	ATP hydrolysis and nucleotide exit enhance maltose translocation in the MalFGK2E importer. Scientific Reports, 2021, 11, 10591.	1.6	1
74	Modeling hydration mechanisms of enzymes in nonpolar and polar organic solvents. FEBS Journal, 2007, .	2.2	0