Claudio M Soares

List of Publications by Year
in descending order

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74 papers	4,010 citations	126708 33 h-index	123241 61 g-index
76 all docs	76 docs citations	76 times ranked	4118 citing authors

#	Article	IF	Citations
1	ATP hydrolysis and nucleotide exit enhance maltose translocation in the MalFGK2E importer. Scientific Reports, 2021, 11, 10591.	1.6	1
2	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
3	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
4	Studying O2 pathways in [NiFe]- and [NiFeSe]-hydrogenases. Scientific Reports, 2020, 10, 10540.	1.6	5
5	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
6	Regulation of the mechanism of Type-II NADH: Quinone oxidoreductase from S. aureus. Redox Biology, 2018, 16, 209-214.	3.9	18
7	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
8	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
9	Structural and Functional insights into the catalytic mechanism of the Type II NADH:quinone oxidoreductase family. Scientific Reports, 2017, 7, 42303.	1.6	22
10	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
11	Structure of Escherichia coli Flavodiiron Nitric Oxide Reductase. Journal of Molecular Biology, 2016, 428, 4686-4707.	2.0	30
12	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
13	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
14	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
15	A molecular perspective on nonaqueous biocatalysis: contributions from simulation studies. Physical Chemistry Chemical Physics, 2013, 15, 13723.	1.3	41
16	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
17	Interaction of Counterions with Subtilisin in Acetonitrile: Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 5838-5848.	1.2	7
18	The Role of Lys147 in the Interaction between MPSA-Gold Nanoparticles and the Î±-Hemolysin Nanopore. Langmuir, 2012, 28, 15643-15650.	1.6	18

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19	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
20	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
21	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
22	Simulation of multihaem cytochromes. FEBS Letters, 2012, 586, 510-518.	1.3	14
23	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
24	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
25	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
26	Nickelâ€“Ironâ€“Selenium Hydrogenases â€“ An Overview. European Journal of Inorganic Chemistry, 2011, 2011, 948-962.	1.0	86
27	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
28	Mechanisms underlying dioxygen reduction in laccases. Structural and modelling studies focusing on proton transfer. BMC Structural Biology, 2010, 10, 28.	2.3	72
29	The multicopper oxidase from the archaeon Pyrobaculumâ€ƒaerophilum shows nitrous oxide reductase activity. FEBS Journal, 2010, 277, 3176-3189.	2.2	48
30	Membrane-Induced Conformational Changes of Kyotorphin Revealed by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 11659-11667.	1.2	21
31	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
32	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
33	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
34	Proton pathways in a [NiFe]â€hydrogenase: A theoretical study. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1010-1022.	1.5	63
35	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
36	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

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37	Modeling hydration mechanisms of enzymes in nonpolar and polar organic solvents. FEBS Journal, 2007, 274, 2424-2436.	2.2	73
38	A robust metallo-oxidase from the hyperthermophilic bacterium Aquifex aeolicus. FEBS Journal, 2007, 274, 2683-2694.	2.2	51
39	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
40	Modeling hydration mechanisms of enzymes in nonpolar and polar organic solvents. FEBS Journal, 2007, .	2.2	0
41	Pathways of H2 toward the Active Site of [NiFe]-Hydrogenase. Biophysical Journal, 2006, 91, 2035-2045.	0.2	66
42	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
43	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
44	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
45	Sulphate respiration from hydrogen in Desulfovibrio bacteria: a structural biology overview. Progress in Biophysics and Molecular Biology, 2005, 89, 292-329.	1.4	141
46	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
47	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
48	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
49	Water Dependent Properties of Cutinase in Nonaqueous Solvents: A Computational Study of Enantioselectivity. Biophysical Journal, 2005, 89, 999-1008.	0.2	38
50	Reorganization and Conformational Changes in the Reduction of Tetraheme Cytochromes. Biophysical Journal, 2005, 89, 3919-3930.	0.2	22
51	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
52	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
53	Modeling Electron Transfer Thermodynamics in Protein Complexes: Interaction between Two Cytochromes c3. Biophysical Journal, 2004, 86, 2773-2785.	0.2	23
54	Docking and electron transfer studies between rubredoxin and rubredoxin:oxygen oxidoreductase. Journal of Biological Inorganic Chemistry, 2003, 8, 475-488.	1.1	20

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55	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
56	Protein Structure and Dynamics in Nonaqueous Solvents: Insights from Molecular Dynamics Simulation Studies. Biophysical Journal, 2003, 84, 1628-1641.	0.2	110
57	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
58	Constant-pH molecular dynamics using stochastic titration. Journal of Chemical Physics, 2002, 117, 4184-4200.	1.2	283
59	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
60	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
61	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
62	[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
63	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
64	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
65	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
66	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
67	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
68	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
69	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
70	An iterative structure-assisted approach to sequence alignment and comparative modeling. , 1999, 37, 55-60.		32
71	Improved modeling of side-chains in proteins with rotamer-based methods: A flexible rotamer model. , 1999, 37, 530-543.		68
72	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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73	Cutinase Activity and Enantioselectivity in Supercritical Fluids. Industrial & Engineering Chemistry Research, 1998, 37, 3189-3194.	1.8	38
74	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