AntÃ³nio M Baptista

List of Publications by Year
in descending order

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91	3,633	136950	149698
papers	citations	32 h-index	56 g-index

98	98	98	3228
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Constant-pH molecular dynamics using stochastic titration. Journal of Chemical Physics, 2002, 117, 4184-4200.	3.0	283
2	Progress in the prediction of pK_a values in proteins. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3260-3275.	2.6	229
3	Simulation of protein conformational freedom as a function of pH: constant-pH molecular dynamics using implicit titration. Proteins: Structure, Function and Bioinformatics, 1997, 27, 523-544.	2.6	162
4	Parametrization of 1-Butyl-3-methylimidazolium Hexafluorophosphate/Nitrate Ionic Liquid for the GROMOS Force Field. Journal of Physical Chemistry B, 2006, 110, 14444-14451.	2.6	131
5	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.	2.6	122
6	Constant-pH Molecular Dynamics with Ionic Strength Effects:Â Protonationâ^'Conformation Coupling in Decalysine. Journal of Physical Chemistry B, 2006, 110, 2927-2933.	2.6	114
7	Protein Structure and Dynamics in Nonaqueous Solvents: Insights from Molecular Dynamics Simulation Studies. Biophysical Journal, 2003, 84, 1628-1641.	0.5	110
8	Simulation of Electron-Proton Coupling with a Monte Carlo Method: Application to Cytochrome c3 Using Continuum Electrostatics. Biophysical Journal, 1999, 76, 2978-2998.	0.5	105
9	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.	2.6	91
10	Characterization of the Protein Unfolding Processes Induced by Urea and Temperature. Biophysical Journal, 2008, 94, 2241-2251.	0.5	85
11	Constant-pH Molecular Dynamics Simulations Reveal a Î²-Rich Form of the Human Prion Protein. Journal of Physical Chemistry B, 2010, 114, 12692-12700.	2.6	83
12	Acidic range titration of HEWL using a constantâ€pH molecular dynamics method. Proteins: Structure, Function and Bioinformatics, 2008, 72, 289-298.	2.6	73
13	Improved modeling of side-chains in proteins with rotamer-based methods: A flexible rotamer model. , 1999, 37, 530-543.		68
14	Pathways of H2 toward the Active Site of [NiFe]-Hydrogenase. Biophysical Journal, 2006, 91, 2035-2045.	0.5	66
15	Lipases and esterases: a review of their sequences, structure and evolution. Biotechnology Annual Review, 1995, 1, 315-371.	2.1	65
16	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.	0.5	63
17	Proton pathways in a [NiFe]â€hydrogenase: A theoretical study. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1010-1022.	2.6	63
18	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

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19	Is the prediction of pK<sub>a</sub values by constantâ€pH molecular dynamics being hindered by inherited problems?. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3437-3447.	2.6	60
20	Molecular Dynamics at Constant pH and Reduction Potential: Application to Cytochrome c₃. Journal of the American Chemical Society, 2009, 131, 12586-12594.	13.7	59
21	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.	2.6	59
22	Reorganization in apo- and holo-Î²-lactoglobulin upon protonation of Glu89: Molecular dynamics and pKa calculations. Proteins: Structure, Function and Bioinformatics, 2004, 54, 744-758.	2.6	50
23	The pH-Dependent Conformational States of Kyotorphin: A Constant-pH Molecular Dynamics Study. Biophysical Journal, 2007, 92, 1836-1845.	0.5	49
24	Conformational Analysis in a Multidimensional Energy Landscape: Study of an Arginylglutamate Repeat. Journal of Physical Chemistry B, 2009, 113, 15989-16001.	2.6	45
25	Structural consequences of ATP hydrolysis on the ABC transporter NBD dimer: Molecular dynamics studies of HlyB. Protein Science, 2011, 20, 1220-1230.	7.6	43
26	Reversibility of Prion Misfolding: Insights from Constant-pH Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 8812-8821.	2.6	41
27	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.	5.4	41
28	A molecular perspective on nonaqueous biocatalysis: contributions from simulation studies. Physical Chemistry Chemical Physics, 2013, 15, 13723.	2.8	41
29	Conformational Component in the Coupled Transfer of Multiple Electrons and Protons in a Monomeric Tetraheme Cytochrome. Journal of Biological Chemistry, 2001, 276, 44044-44051.	3.4	39
30	The lactate dehydrogenases encoded by the ldh and ldhB genes in Lactococcus lactis exhibit distinct regulation and catalytic propertiesâ€ƒâ€”â€ƒcomparative modeling to probe the molecular basis. FEBS Journal, 2007, 274, 5924-5936.	4.7	39
31	Water Dependent Properties of Cutinase in Nonaqueous Solvents: A Computational Study of Enantioselectivity. Biophysical Journal, 2005, 89, 999-1008.	0.5	38
32	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.	2.6	37
33	Constant-pH MD Simulations of DMPA/DMPC Lipid Bilayers. Journal of Chemical Theory and Computation, 2015, 11, 5973-5979.	5.3	36
34	Unfolding the Conformational Behavior of Peptide Dendrimers: Insights from Molecular Dynamics Simulations. Journal of the American Chemical Society, 2011, 133, 5042-5052.	13.7	34
35	Molecular Anatomy of Plant Photoprotective Switches: The Sensitivity of PsbS to the Environment, Residue by Residue. Journal of Physical Chemistry Letters, 2019, 10, 1737-1742.	4.6	34
36	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.	2.6	31

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37	Constant-pH MD Simulations of an Oleic Acid Bilayer. Journal of Chemical Theory and Computation, 2015, 11, 2367-2376.	5.3	30
38	Protonation of DMPC in a Bilayer Environment Using a Linear Response Approximation. Journal of Chemical Theory and Computation, 2014, 10, 2176-2184.	5.3	29
39	Inter-domain Communication Mechanisms in an ABC Importer: A Molecular Dynamics Study of the MalFGK2E Complex. PLoS Computational Biology, 2011, 7, e1002128.	3.2	28
40	Predicting the Thermodynamics and Kinetics of Helix Formation in a Cyclic Peptide Model. Journal of Chemical Theory and Computation, 2013, 9, 5148-5157.	5.3	28
41	Protein Electrostatics. Biotechnology Annual Review, 1996, 2, 315-372.	2.1	27
42	Structural Effects of pH and Deacylation on Surfactant Protein C in an Organic Solvent Mixture: A Constant-pH MD Study. Journal of Chemical Information and Modeling, 2013, 53, 2979-2989.	5.4	26
43	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.	3.4	25
44	Comment on â€œExplicit-solvent molecular dynamics simulation at constant pH: Methodology and application to small aminesâ€•[J. Chem. Phys. 114, 9706 (2001)]. Journal of Chemical Physics, 2002, 116, 7766-7768.	3.0	24
45	The blind watchmaker and rational protein engineering. Journal of Biotechnology, 1994, 36, 185-220.	3.8	23
46	Modeling Electron Transfer Thermodynamics in Protein Complexes: Interaction between Two Cytochromes c3. Biophysical Journal, 2004, 86, 2773-2785.	0.5	23
47	Redox Properties of Thermus thermophilus ba3: Different Electron-Proton Coupling in Oxygen Reductases?. Biophysical Journal, 2008, 94, 2434-2441.	0.5	23
48	Treatment of Ionic Strength in Biomolecular Simulations of Charged Lipid Bilayers. Journal of Chemical Theory and Computation, 2014, 10, 5483-5492.	5.3	23
49	Reorganization and Conformational Changes in the Reduction of Tetraheme Cytochromes. Biophysical Journal, 2005, 89, 3919-3930.	0.5	22
50	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.	3.2	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.	2.6	21
52	Membrane-Induced Conformational Changes of Kyotorphin Revealed by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 11659-11667.	2.6	21
53	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.	2.6	20
54	Coupling between protonation and conformation in cytochrome c oxidase: Insights from constant-pH MD simulations. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 759-771.	1.0	20

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55	Role of Counterions in Constant-pH Molecular Dynamics Simulations of PAMAM Dendrimers. ACS Omega, 2018, 3, 2001-2009.	3.5	20
56	Predicting protein partition coefficients in aqueous two phase system. Journal of Chromatography A, 2016, 1470, 50-58.	3.7	19
57	Cerebrovascular changes in rats during ischemia and reperfusion: A comparison of bold and first pass bolus tracking techniques. Magnetic Resonance in Medicine, 1996, 35, 489-496.	3.0	18
58	The Origin of Trypsin: Evidence for Multiple Gene Duplications in Trypsins. Journal of Molecular Evolution, 1998, 47, 353-362.	1.8	18
59	Thermodynamic Redox Behavior of the Heme Centers of cbb₃ Heme-Copper Oxygen Reductase from Bradyrhizobium japonicum. Biochemistry, 2007, 46, 13245-13253.	2.5	18
60	Conformational and dynamics changes induced by bile acids binding to chicken liver bile acid binding protein. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1889-1898.	2.6	18
61	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.	2.6	18
62	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.	2.6	17
63	Modeling the partitioning of amino acids in aqueous two phase systems. Journal of Chromatography A, 2014, 1329, 52-60.	3.7	17
64	Constant-pH Molecular Dynamics Study of Kyotorphin in an Explicit Bilayer. Biophysical Journal, 2015, 108, 2282-2290.	0.5	17
65	A pH Replica Exchange Scheme in the Stochastic Titration Constant-pH MD Method. Journal of Chemical Theory and Computation, 2019, 15, 3108-3116.	5.3	17
66	Predicting the partition coefficients of a recombinant cutinase in polyethylene glycol/phosphate aqueous two-phase systems. , 1997, 56, 248-257.		16
67	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.	2.9	16
68	Exploring the Structural Properties of Positively Charged Peptide Dendrimers. Journal of Physical Chemistry B, 2016, 120, 11323-11330.	2.6	16
69	Improving protein extraction yield in reversed micellar systems through surface charge engineering. Biotechnology and Bioengineering, 1994, 44, 773-780.	3.3	15
70	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.	5.3	15
71	Simulation of multihaem cytochromes. FEBS Letters, 2012, 586, 510-518.	2.8	14
72	Effect of pH on the influenza fusion peptide properties unveiled by constant-pH molecular dynamics simulations combined with experiment. Scientific Reports, 2020, 10, 20082.	3.3	14

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73	Structural determinants of ligand imprinting: A molecular dynamics simulation study of subtilisin in aqueous and apolar solvents. Protein Science, 2011, 20, 379-386.	7.6	13
74	The Effect of Membrane Environment on Surfactant Protein C Stability Studied by Constant-pH Molecular Dynamics. Journal of Chemical Information and Modeling, 2015, 55, 2206-2217.	5.4	13
75	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.	2.5	12
76	Photonic Activation of Plasminogen Induced by Low Dose UVB. PLoS ONE, 2015, 10, e0116737.	2.5	12
77	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.	5.4	9
78	Theoretical Identification of Proton Channels in the Quinol Oxidase aa3 from Acidianus ambivalens. Biophysical Journal, 2004, 87, 4316-4325.	0.5	8
79	Structuring Peptide Dendrimers through pH Modulation and Substrate Binding. Journal of Physical Chemistry B, 2016, 120, 10138-10152.	2.6	8
80	Interaction of Counterions with Subtilisin in Acetonitrile: Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 5838-5848.	2.6	7
81	Water Encapsulation in a Polyoxapolyaza Macrobicyclic Compound. Journal of Organic Chemistry, 2012, 77, 6816-6824.	3.2	7
82	Unraveling the Conformational Determinants of Peptide Dendrimers Using Molecular Dynamics Simulations. Macromolecules, 2013, 46, 9427-9436.	4.8	7
83	The anti-inflammatory action of the analgesic kyotorphin neuropeptide derivatives: insights of a lipid-mediated mechanism. Amino Acids, 2016, 48, 307-318.	2.7	7
84	Approach to Study pH-Dependent Protein Association Using Constant-pH Molecular Dynamics: Application to the Dimerization of Î²-Lactoglobulin. Journal of Chemical Theory and Computation, 2022, 18, 1982-2001.	5.3	7
85	Thermodynamic Redox Behavior of the Heme Centers in A-Type Heme-Copper Oxygen Reductases: Comparison between the Two Subfamilies. Biophysical Journal, 2008, 95, 4448-4455.	0.5	6
86	A Study of the Contribution of Changes in the Cerebral Blood Volume to the Haemodynamic Response to Anoxia in Rat Brain. NMR in Biomedicine, 1996, 9, 233-240.	2.8	5
87	A Study of the contribution of changes in the cerebral blood volume to the haemodynamic response to anoxia in rat brain. , 1997, 10, 59-66.		5
88	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.	5.4	5
89	Simulation of protein conformational freedom as a function of pH: constantâ€pH molecular dynamics using implicit titration. Proteins: Structure, Function and Bioinformatics, 1997, 27, 523-544.	2.6	4
90	Electrostatic studies of carbohydrate active enzymes. Progress in Biotechnology, 1995, 10, 181-204.	0.2	1

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91	Constant-pH MD Simulations Portray the Protonation and Structural Behavior of Four Decapeptides Designed to Coordinate Cu²⁺. Journal of Physical Chemistry B, 2016, 120, 1080-1091.	2.6	1