AntÃ³nio M Baptista

List of Publications by Year
in descending order

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91 papers	3,633 citations	136885 32 h-index	149623 56 g-index
98 all docs	98 docs citations	98 times ranked	3228 citing authors

#	Article	IF	Citations
1	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.	2.3	7
2	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
3	A pH Replica Exchange Scheme in the Stochastic Titration Constant-pH MD Method. Journal of Chemical Theory and Computation, 2019, 15, 3108-3116.	2.3	17
4	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.	2.1	34
5	Role of Counterions in Constant-pH Molecular Dynamics Simulations of PAMAM Dendrimers. ACS Omega, 2018, 3, 2001-2009.	1.6	20
6	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
7	Structuring Peptide Dendrimers through pH Modulation and Substrate Binding. Journal of Physical Chemistry B, 2016, 120, 10138-10152.	1.2	8
8	Predicting protein partition coefficients in aqueous two phase system. Journal of Chromatography A, 2016, 1470, 50-58.	1.8	19
9	Exploring the Structural Properties of Positively Charged Peptide Dendrimers. Journal of Physical Chemistry B, 2016, 120, 11323-11330.	1.2	16
10	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.	1.2	1
11	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
12	The anti-inflammatory action of the analgesic kyotorphin neuropeptide derivatives: insights of a lipid-mediated mechanism. Amino Acids, 2016, 48, 307-318.	1.2	7
13	Photonic Activation of Plasminogen Induced by Low Dose UVB. PLoS ONE, 2015, 10, e0116737.	1.1	12
14	Constant-pH MD Simulations of an Oleic Acid Bilayer. Journal of Chemical Theory and Computation, 2015, 11, 2367-2376.	2.3	30
15	Constant-pH Molecular Dynamics Study of Kyotorphin in an Explicit Bilayer. Biophysical Journal, 2015, 108, 2282-2290.	0.2	17
16	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.	2.5	13
17	Constant-pH MD Simulations of DMPA/DMPC Lipid Bilayers. Journal of Chemical Theory and Computation, 2015, 11, 5973-5979.	2.3	36
18	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

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19	Treatment of Ionic Strength in Biomolecular Simulations of Charged Lipid Bilayers. Journal of Chemical Theory and Computation, 2014, 10, 5483-5492.	2.3	23
20	Protonation of DMPC in a Bilayer Environment Using a Linear Response Approximation. Journal of Chemical Theory and Computation, 2014, 10, 2176-2184.	2.3	29
21	Modeling the partitioning of amino acids in aqueous two phase systems. Journal of Chromatography A, 2014, 1329, 52-60.	1.8	17
22	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
23	A molecular perspective on nonaqueous biocatalysis: contributions from simulation studies. Physical Chemistry Chemical Physics, 2013, 15, 13723.	1.3	41
24	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.	2.5	26
25	Unraveling the Conformational Determinants of Peptide Dendrimers Using Molecular Dynamics Simulations. Macromolecules, 2013, 46, 9427-9436.	2.2	7
26	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
27	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
28	Interaction of Counterions with Subtilisin in Acetonitrile: Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 5838-5848.	1.2	7
29	Reversibility of Prion Misfolding: Insights from Constant-pH Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 8812-8821.	1.2	41
30	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
31	Water Encapsulation in a Polyoxapolyaza Macrobicyclic Compound. Journal of Organic Chemistry, 2012, 77, 6816-6824.	1.7	7
32	Simulation of multihaem cytochromes. FEBS Letters, 2012, 586, 510-518.	1.3	14
33	Unfolding the Conformational Behavior of Peptide Dendrimers: Insights from Molecular Dynamics Simulations. Journal of the American Chemical Society, 2011, 133, 5042-5052.	6.6	34
34	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
35	Is the prediction of pK_avalues by constantâ€pH molecular dynamics being hindered by inherited problems?. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3437-3447.	1.5	60
36	Progress in the prediction of pK_a values in proteins. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3260-3275.	1.5	229

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37	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
38	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
39	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
40	Membrane-Induced Conformational Changes of Kyotorphin Revealed by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 11659-11667.	1.2	21
41	Constant-pH Molecular Dynamics Simulations Reveal a Î²-Rich Form of the Human Prion Protein. Journal of Physical Chemistry B, 2010, 114, 12692-12700.	1.2	83
42	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
43	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
44	Molecular Dynamics at Constant pH and Reduction Potential: Application to Cytochrome c₃. Journal of the American Chemical Society, 2009, 131, 12586-12594.	6.6	59
45	Conformational Analysis in a Multidimensional Energy Landscape: Study of an Arginylglutamate Repeat. Journal of Physical Chemistry B, 2009, 113, 15989-16001.	1.2	45
46	Proton pathways in a [NiFe]â€hydrogenase: A theoretical study. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1010-1022.	1.5	63
47	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.	1.5	18
48	Acidic range titration of HEWL using a constantâ€pH molecular dynamics method. Proteins: Structure, Function and Bioinformatics, 2008, 72, 289-298.	1.5	73
49	Characterization of the Protein Unfolding Processes Induced by Urea and Temperature. Biophysical Journal, 2008, 94, 2241-2251.	0.2	85
50	Redox Properties of Thermus thermophilus ba3: Different Electron-Proton Coupling in Oxygen Reductases?. Biophysical Journal, 2008, 94, 2434-2441.	0.2	23
51	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.	0.2	6
52	Thermodynamic Redox Behavior of the Heme Centers of cbb₃ Heme-Copper Oxygen Reductase from Bradyrhizobium japonicum. Biochemistry, 2007, 46, 13245-13253.	1.2	18
53	The pH-Dependent Conformational States of Kyotorphin: A Constant-pH Molecular Dynamics Study. Biophysical Journal, 2007, 92, 1836-1845.	0.2	49
54	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.	2.2	39

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55	Constant-pH Molecular Dynamics with Ionic Strength Effects:Â Protonationâ^'Conformation Coupling in Decalysine. Journal of Physical Chemistry B, 2006, 110, 2927-2933.	1.2	114
56	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
57	Pathways of H2 toward the Active Site of [NiFe]-Hydrogenase. Biophysical Journal, 2006, 91, 2035-2045.	0.2	66
58	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
59	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
60	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
61	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
62	Water Dependent Properties of Cutinase in Nonaqueous Solvents: A Computational Study of Enantioselectivity. Biophysical Journal, 2005, 89, 999-1008.	0.2	38
63	Reorganization and Conformational Changes in the Reduction of Tetraheme Cytochromes. Biophysical Journal, 2005, 89, 3919-3930.	0.2	22
64	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
65	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.	1.5	50
66	Theoretical Identification of Proton Channels in the Quinol Oxidase aa3 from Acidianus ambivalens. Biophysical Journal, 2004, 87, 4316-4325.	0.2	8
67	Modeling Electron Transfer Thermodynamics in Protein Complexes: Interaction between Two Cytochromes c3. Biophysical Journal, 2004, 86, 2773-2785.	0.2	23
68	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
69	Protein Structure and Dynamics in Nonaqueous Solvents: Insights from Molecular Dynamics Simulation Studies. Biophysical Journal, 2003, 84, 1628-1641.	0.2	110
70	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
71	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.	1.2	24
72	Constant-pH molecular dynamics using stochastic titration. Journal of Chemical Physics, 2002, 117, 4184-4200.	1.2	283

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73	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
74	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
75	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
76	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
77	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
78	Improved modeling of side-chains in proteins with rotamer-based methods: A flexible rotamer model. , 1999, 37, 530-543.		68
79	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
80	The Origin of Trypsin: Evidence for Multiple Gene Duplications in Trypsins. Journal of Molecular Evolution, 1998, 47, 353-362.	0.8	18
81	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
82	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.	1.5	162
83	Predicting the partition coefficients of a recombinant cutinase in polyethylene glycol/phosphate aqueous two-phase systems. , 1997, 56, 248-257.		16
84	Simulation of protein conformational freedom as a function of pH: constant-pH molecular dynamics using implicit titration. , 1997, 27, 523.		4
85	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.	1.6	5
86	Protein Electrostatics. Biotechnology Annual Review, 1996, 2, 315-372.	2.1	27
87	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.	1.9	18
88	Electrostatic studies of carbohydrate active enzymes. Progress in Biotechnology, 1995, 10, 181-204.	0.2	1
89	Lipases and esterases: a review of their sequences, structure and evolution. Biotechnology Annual Review, 1995, 1, 315-371.	2.1	65
90	Improving protein extraction yield in reversed micellar systems through surface charge engineering. Biotechnology and Bioengineering, 1994, 44, 773-780.	1.7	15

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91	The blind watchmaker and rational protein engineering. Journal of Biotechnology, 1994, 36, 185-220.	1.9	23