VÃ-tor H Teixeira

List of Publications by Year
in descending order

23 papers	1,085 citations	430874 18 h-index	642732 23 g-index
23 all docs	23 docs citations	23 times ranked	1348 citing authors

#	Article	IF	Citations
1	The role of electrostatics in TrxR electron transfer mechanism: A computational approach. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1836-1843.	2.6	10
2	pK_a Values of Titrable Amino Acids at the Water/Membrane Interface. Journal of Chemical Theory and Computation, 2016, 12, 930-934.	5.3	59
3	Molecular Details of INH-C₁₀ Binding to wt KatG and Its S315T Mutant. Molecular Pharmaceutics, 2015, 12, 898-909.	4.6	12
4	Constant-pH MD Simulations of an Oleic Acid Bilayer. Journal of Chemical Theory and Computation, 2015, 11, 2367-2376.	5.3	30
5	Constant-pH MD Simulations of DMPA/DMPC Lipid Bilayers. Journal of Chemical Theory and Computation, 2015, 11, 5973-5979.	5.3	36
6	Treatment of Ionic Strength in Biomolecular Simulations of Charged Lipid Bilayers. Journal of Chemical Theory and Computation, 2014, 10, 5483-5492.	5.3	23
7	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
8	One-Electron Oxidation of ReCp(CO)₂L (L = PPh₃, Î·²-2-Butene,) Tj ETQq0 0 0 rgBT /Overlock 10 Properties and Dimerization Tendencies of 17-Electron Rhenium Complexes. Organometallics, 2014, 33, 4706-4715.	2.3	5
9	Tuning the Bioactivity of Tensioactive Deoxy Glycosides to Structure: Antibacterial Activity Versus Selective Cholinesterase Inhibition Rationalized by Molecular Docking. European Journal of Organic Chemistry, 2013, 2013, 1448-1459.	2.4	7
10	Conformational Study of GSH and GSSG Using Constant-pH Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 7507-7517.	2.6	29
11	Structural features of [NiFeSe] and [NiFe] hydrogenases determining their different properties: a computational approach. Journal of Biological Inorganic Chemistry, 2012, 17, 543-555.	2.6	26
12	Analysis of binding modes of ligands to multiple conformations of CYP3A4. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2010, 1804, 2036-2045.	2.3	25
13	Proton pathways in a [NiFe]â€hydrogenase: A theoretical study. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1010-1022.	2.6	63
14	Pathways of H2 toward the Active Site of [NiFe]-Hydrogenase. Biophysical Journal, 2006, 91, 2035-2045.	0.5	66
15	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
16	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
17	Water Dependent Properties of Cutinase in Nonaqueous Solvents: A Computational Study of Enantioselectivity. Biophysical Journal, 2005, 89, 999-1008.	0.5	38
18	Reorganization and Conformational Changes in the Reduction of Tetraheme Cytochromes. Biophysical Journal, 2005, 89, 3919-3930.	0.5	22

#	Article	IF	Citations
19	Modeling Electron Transfer Thermodynamics in Protein Complexes: Interaction between Two Cytochromes c3. Biophysical Journal, 2004, 86, 2773-2785.	0.5	23
20	Protein Structure and Dynamics in Nonaqueous Solvents: Insights from Molecular Dynamics Simulation Studies. Biophysical Journal, 2003, 84, 1628-1641.	0.5	110
21	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
22	Constant-pH molecular dynamics using stochastic titration. Journal of Chemical Physics, 2002, 117, 4184-4200.	3.0	283
23	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