SÃ-lvia G. EstÃ¡cio

List of Publications by Year
in descending order

17 papers	388 citations	933447 10 h-index	839539 18 g-index
18 all docs	18 docs citations	18 times ranked	556 citing authors

#	Article	IF	Citations
1	Energetics of Intramolecular Hydrogen Bonding in Di-substituted Benzenes by the orthoâ^'para Method. Journal of Physical Chemistry A, 2004, 108, 10834-10843.	2.5	94
2	The Kohn-Sham density of states and band gap of water: From small clusters to liquid water. Journal of Chemical Physics, 2005, 123, 054510.	3.0	52
3	Identification of a Conserved Aggregation-Prone Intermediate State in the Folding Pathways of Spc-SH3 Amyloidogenic Variants. Journal of Molecular Biology, 2012, 422, 705-722.	4.2	43
4	A Simulated Intermediate State for Folding and Aggregation Provides Insights into Î"N6 Î²2-Microglobulin Amyloidogenic Behavior. PLoS Computational Biology, 2014, 10, e1003606.	3.2	34
5	Robustness of atomistic GÅ•models in predicting native-like folding intermediates. Journal of Chemical Physics, 2012, 137, 085102.	3.0	30
6	Bornâ€"Oppenheimer molecular dynamics of phenol in a water cluster. Chemical Physics Letters, 2008, 456, 170-175.	2.6	19
7	Assessing the Effect of Loop Mutations in the Folding Space of Î²2-Microglobulin with Molecular Dynamics Simulations. International Journal of Molecular Sciences, 2013, 14, 17256-17278.	4.1	17
8	Câ^'H Bond Dissociation Enthalpies in Norbornane. An Experimental and Computational Study. Organic Letters, 2008, 10, 1613-1616.	4.6	16
9	Calcium binding to gatekeeper residues flanking aggregation-prone segments underlies non-fibrillar amyloid traits in superoxide dismutase 1 (SOD1). Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 118-126.	2.3	13
10	Thermal unfolding simulations of NBD1 domain variants reveal structural motifs associated with the impaired folding of F508del-CFTR. Molecular BioSystems, 2016, 12, 2834-2848.	2.9	13
11	Reaction ofpara-Hydroxy-Substituted Diphenylmethanes withtert-Butoxy Radical. ChemPhysChem, 2004, 5, 1217-1221.	2.1	12
12	Structureâ€based virtual screening toward the discovery of novel inhibitors of the <scp>DNA</scp> repair activity of the human apurinic/apyrimidinic endonuclease 1. Chemical Biology and Drug Design, 2016, 88, 915-925.	3.2	9
13	Characterizing the Dynamics and Ligand-Specific Interactions in the Human Leukocyte Elastase through Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2011, 51, 1690-1702.	5.4	8
14	Homolytic dissociation in hydrogen-bonding liquids: energetics of the phenol O?H bond in methanol and the water O?H bond in water. Theoretical Chemistry Accounts, 2004, 112, 282.	1.4	7
15	Energetics of tert-Butoxyl Addition Reaction to Norbornadiene: A Method for Estimating the Ï€-Bond Strength of a Carbonâ^'Carbon Double Bond. Journal of Physical Chemistry A, 2009, 113, 6524-6530.	2.5	4
16	In Silico Strategies Toward Enzyme Function and Dynamics. Advances in Protein Chemistry and Structural Biology, 2012, 87, 249-292.	2.3	3
17	Electronic Properties of Hydrogen Bond Networks: Implications for Solvent Effects in Polar Liquids. Challenges and Advances in Computational Chemistry and Physics, 2008, , 115-133.	0.6	2