OtÃ¡vio LuÃ-s de Santana

List of Publications by Year
in descending order

10 papers	66 citations	2258059 3 h-index	1720034 7 g-index
10 all docs	10 docs citations	10 times ranked	97 citing authors

#	Article	IF	Citations
1	Diradicalar Character and Ring Stability of Mesoionic Heterocyclic Oxazoles and Thiazoles by Ab Initio Mono and Multi-Reference Methods. Molecules, 2020, 25, 4524.	3.8	0
2	A multireference configuration interaction study with singles and doubles of some mesoionic rings: reaction and activation free energies for the ringâ€opening reaction. International Journal of Quantum Chemistry, 2020, 120, e26391.	2.0	0
3	One-Electron Reduction Potentials: Calibration of Theoretical Protocols for Moritaâ€“Baylisâ€“Hillman Nitroaromatic Compounds in Aprotic Media. Molecules, 2018, 23, 2129.	3.8	3
4	Challenges encountered during development of Mn porphyrin-based, potent redox-active drug and superoxide dismutase mimic, MnTnBuOE-2-PyP5+, and its alkoxyalkyl analogues. Journal of Inorganic Biochemistry, 2017, 169, 50-60.	3.5	18
5	Electronic properties of the low-lying spin states of dimethylnitrosamine coordinated to Fe(III) heme models: An ab initio study. International Journal of Quantum Chemistry, 2014, 114, 508-520.	2.0	2
6	Theoretical calculations of the substituent effect on molecular properties of the RCNâ¯HF hydrogen-bonded complexes with R=NH2, CH3O, CH3, OH, SH, H, Cl, F, CF3, CN and NO2. Vibrational Spectroscopy, 2009, 49, 133-141.	2.2	3
7	O ensino de reaÃ§Ãµes orgÃ¢nicas usando quÃmica computacional: I. reaÃ§Ãµes de adiÃ§Ã£o eletrofÃlica a alquenos. Quimica Nova, 2008, 31, 1243-1249.	0.3	1
8	Theoretical study of cooperative effects in the homo- and heteromeric hydrogen bond chains (HCN)nï£¿HF withn = 1, 2, and 3. International Journal of Quantum Chemistry, 2006, 106, 2714-2722.	2.0	29
9	Green's function calculation of through-bond electronic coupling in donor-bridge-acceptor model systems II: Importance factors applied to atomic sites. International Journal of Quantum Chemistry, 2005, 102, 265-274.	2.0	0
10	Green's function calculation of through-bond electronic coupling in donorâ€“bridgeâ€“acceptor model systems. Chemical Physics Letters, 1999, 314, 508-515.	2.6	10