Chinnasamy Kalaiarasi

List of Publications by Year
in descending order

14 papers	124 citations	1307594 7 h-index	1281871 11 g-index
17 all docs	17 docs citations	17 times ranked	202 citing authors

#	Article	IF	Citations
1	Understanding the conformational flexibility and electrostatic properties of curcumin in the active site of rhAChE via molecular docking, molecular dynamics, and charge density analysis. Journal of Biomolecular Structure and Dynamics, 2017, 35, 3627-3647.	3.5	26
2	Topological characterization of electron density, electrostatic potential and intermolecular interactions of 2-nitroimidazole: an experimental and theoretical study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 775-786.	1.1	23
3	Charge density and electrostatic potential of hepatitis C anti-viral agent andrographolide: an experimental and theoretical study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2018, 74, 693-704.	1.1	11
4	Experimental and theoretical charge density, intermolecular interactions and electrostatic properties of metronidazole. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 942-953.	1.1	10
5	Crystal structure and theoretical charge density studies of dilantin molecule. Journal of Molecular Structure, 2018, 1170, 105-118.	3.6	8
6	Evaluation of binding and antagonism/downregulation of brilanestrant molecule in estrogen receptor-Î± via quantum mechanics/molecular mechanics, molecular dynamics and binding free energy calculations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 219-235.	3.5	8
7	Topology of electron density and electrostatic potential of HIV reverse transcriptase inhibitor zidovudine from high resolution X-ray diffraction and charge density analysis. Journal of Molecular Structure, 2019, 1180, 683-697.	3.6	7
8	Investigation of binding mechanism and downregulation of elacestrant for wild and L536S mutant estrogen receptorâ€Î± through molecular dynamics simulation and binding free energy analysis. Journal of Computational Chemistry, 2020, 41, 97-109.	3.3	7
9	Strong Binding of Leupeptin with TMPRSS2 Protease May Be an Alternative to Camostat and Nafamostat for SARS-CoV-2 Repurposed Drug: Evaluation from Molecular Docking and Molecular Dynamics Simulations. Applied Biochemistry and Biotechnology, 2021, 193, 1909-1923.	2.9	7
10	Structure and charge density distribution of amine azide based hypergolic propellant molecules: a theoretical study. Canadian Journal of Chemistry, 2016, 94, 126-136.	1.1	5
11	Combined quantum mechanics/molecular mechanics (QM/MM) methods to understand the charge density distribution of estrogens in the active site of estrogen receptors. RSC Advances, 2019, 9, 40758-40771.	3.6	5
12	Synthesis and Antibacterial Activity of New Nâ€Substituted Hexahydroquinolinone Derivatives and Xâ€Ray Crystallographic Studies. ChemistrySelect, 2020, 5, 2696-2700.	1.5	3
13	Intermolecular interactions and charge density distribution of endocrine-disrupting molecules (xenoestrogens) with ERÎ±: QM/MM perspective. Structural Chemistry, 2020, 31, 1013-1028.	2.0	2
14	Investigation of bond topological and electrostatic properties of plumbagin molecule: An experimental and theoretical charge density study. Journal of Molecular Structure, 2020, 1220, 128714.	3.6	2