

Konda Reddy Karnati

List of Publications by Year in descending order

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papers

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949033

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docs citations

16
times ranked

471
citing authors

#	ARTICLE	IF	CITATIONS
1	Mechanistic Insights into SARS-CoV-2 Main Protease Inhibition Reveals Hotspot Residues. Journal of Chemical Information and Modeling, 2021, , .	2.5	5
2	Exploring the binding mode and thermodynamics of inverse agonists against estrogen-related receptor alpha. RSC Advances, 2020, 10, 16659-16668.	1.7	2
3	Structural and binding insights into HIV-1 protease and P2-ligand interactions through molecular dynamics simulations, binding free energy and principal component analysis. Journal of Molecular Graphics and Modelling, 2019, 92, 112-122.	1.3	11
4	A fluorescence-displacement assay using molecularly imprinted polymers for the visual, rapid, and sensitive detection of the algal metabolites, geosmin and 2-methylisoborneol. Analytica Chimica Acta, 2019, 1066, 121-130.	2.6	15
5	Understanding the co-loading and releasing of doxorubicin and paclitaxel using chitosan functionalized single-walled carbon nanotubes by molecular dynamics simulations. Physical Chemistry Chemical Physics, 2018, 20, 9389-9400.	1.3	78
6	Effect of HIV-1 Subtype C integrase mutations implied using molecular modeling and docking data. Bioinformation, 2016, 12, 221-230.	0.2	5
7	Insight into the Binding Mode between N-Methyl Pyrimidones and Prototype Foamy Virus Integrase-DNA Complex by QM-Polarized Ligand Docking and Molecular Dynamics Simulations. Current Topics in Medicinal Chemistry, 2015, 15, 43-49.	1.0	8
8	Combined ligand and structure-based approaches on HIV-1 integrase strand transfer inhibitors. Chemico-Biological Interactions, 2014, 218, 71-81.	1.7	29
9	Blocking the interaction between HIV-1 integrase and human LEDGF/p75: mutational studies, virtual screening and molecular dynamics simulations. Molecular BioSystems, 2014, 10, 526.	2.9	32
10	A three-dimensional chemical phase pharmacophore mapping, QSAR modelling and electronic feature analysis of benzofuran salicylic acid derivatives as LYP inhibitors. SAR and QSAR in Environmental Research, 2013, 24, 1025-1040.	1.0	14
11	Identification of potential HIV-1 integrase strand transfer inhibitors: <i>in silico</i> virtual screening and QM/MM docking studies. SAR and QSAR in Environmental Research, 2013, 24, 581-595.	1.0	33
12	Shape and pharmacophore-based virtual screening to identify potential cytochrome P450 sterol 14 α -demethylase inhibitors. Journal of Receptor and Signal Transduction Research, 2013, 33, 234-243.	1.3	32
13	Molecular docking, QPLD, and ADME prediction studies on HIV-1 integrase leads. Medicinal Chemistry Research, 2012, 21, 4239-4251.	1.1	28
14	In silico screening of indinavir-based compounds targeting proteolytic activity in HIV PR: binding pocket fit approach. Medicinal Chemistry Research, 2012, 21, 4060-4068.	1.1	33
15	Exploring the selectivity of a ligand complex with CDK2/CDK1: a molecular dynamics simulation approach. Journal of Molecular Recognition, 2012, 25, 504-512.	1.1	39
16	Pharmacophore modelling and atom-based 3D-QSAR studies on <i>N</i> -methyl pyrimidones as HIV-1 integrase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2012, 27, 339-347.	2.5	33