# Konda Reddy Karnati

List of Publications by Year
in descending order



| 16 | 397 | 840776 11 | 940533 16 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 16 | 16 | 16 | 426 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | 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. | 2.8 | 78 |
| 2 | Exploring the selectivity of a ligand complex with CDK2/CDK1: a molecular dynamics simulation approach. Journal of Molecular Recognition, 2012, 25, 504-512. | 2.1 | 39 |
| 3 | In silico screening of indinavir-based compounds targeting proteolytic activity in HIV PR: binding pocket fit approach. Medicinal Chemistry Research, 2012, 21, 4060-4068. | 2.4 | 33 |
| 4 | Pharmacophore modelling and atom-based 3D-QSAR studies on N-methyl pyrimidones as HIV-1 integrase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2012, 27, 339-347. | 5.2 | 33 |
| 5 | Identification of potential HIV-1 integrase strand transfer inhibitors:In silicovirtual screening and QM/MM docking studies. SAR and QSAR in Environmental Research, 2013, 24, 581-595. | 2.2 | 33 |
| 6 | Shape and pharmacophore-based virtual screening to identify potential cytochrome P450 sterol 14Î±-demethylase inhibitors. Journal of Receptor and Signal Transduction Research, 2013, 33, 234-243. | 2.5 | 32 |
| 7 | 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 |
| 8 | Combined ligand and structure-based approaches on HIV-1 integrase strand transfer inhibitors. Chemico-Biological Interactions, 2014, 218, 71-81. | 4.0 | 29 |
| 9 | Molecular docking, QPLD, and ADME prediction studies on HIV-1 integrase leads. Medicinal Chemistry Research, 2012, 21, 4239-4251. | 2.4 | 28 |
| 10 | 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. | 5.4 | 15 |
| 11 | 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. | 2.2 | 14 |
| 12 | 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. | 2.4 | 11 |
| 13 | 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. | 2.1 | 8 |
| 14 | Effect of HIV-1 Subtype C integrase mutations implied using molecular modeling and docking data. Bioinformation, 2016, 12, 221-230. | 0.5 | 5 |
| 15 | Mechanistic Insights into SARS-CoV-2 Main Protease Inhibition Reveals Hotspot Residues. Journal of Chemical Information and Modeling, 2021, , . | 5.4 | 5 |
| 16 | Exploring the binding mode and thermodynamics of inverse agonists against estrogen-related receptor alpha. RSC Advances, 2020, 10, 16659-16668. | 3.6 | 2 |