Daniel M Shadrack

List of Publications by Year
in descending order

20 papers	158 citations	1307594 7 h-index	1199594 12 g-index
20 all docs	20 docs citations	20 times ranked	208 citing authors

#	Article	IF	Citations
1	Polyamidoamine Dendrimers for Enhanced Solubility of Small Molecules and Other Desirable Properties for Site Specific Delivery: Insights from Experimental and Computational Studies. Molecules, 2018, 23, 1419.	3.8	36
2	Synthesis of Polyamidoamine Dendrimer for Encapsulating Tetramethylscutellarein for Potential Bioactivity Enhancement. International Journal of Molecular Sciences, 2015, 16, 26363-26377.	4.1	31
3	Luteolin: a blocker of SARS-CoV-2 cell entry based on relaxed complex scheme, molecular dynamics simulation, and metadynamics. Journal of Molecular Modeling, 2021, 27, 221.	1.8	17
4	A computational study on the role of water and conformational fluctuations in Hsp90 in response to inhibitors. Journal of Molecular Graphics and Modelling, 2020, 96, 107510.	2.4	12
5	Crystal structure and Hirshfeld surface analysis of (E)-4-{2,2-dichloro-1-[(3,5-dimethylphenyl)diazenyl]ethenyl}-N,N-dimethylaniline. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1251-1254.	0.5	8
6	Solvent effects on molecular encapsulation of Toussantine-A by chitosan nanoparticle: A metadynamics study. Journal of Molecular Liquids, 2019, 292, 111434.	4.9	7
7	In silico study of the inhibition of SARS-COV-2 viral cell entry by neem tree extracts. RSC Advances, 2021, 11, 26524-26533.	3.6	7
8	Ensemble-based screening of natural products and FDA-approved drugs identified potent inhibitors of SARS-CoV-2 that work with two distinct mechanisms. Journal of Molecular Graphics and Modelling, 2021, 105, 107871.	2.4	7
9	Hydrophobic Ï€-Ï€ stacking interactions and hydrogen bonds drive self-aggregation of luteolin in water. Journal of Molecular Graphics and Modelling, 2022, 116, 108243.	2.4	6
10	Molecular dynamics simulation of bioactive compounds of Withania somnifera leaf extract as DNA gyrase inhibitor. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9279-9286.	3.5	5
11	Cationâ€“Ï€ interactions drive hydrophobic self-assembly and aggregation of niclosamide in water. RSC Advances, 2021, 11, 33136-33147.	3.6	5
12	Finding alternatives to 5-fluorouracil: application of ensemble-based virtual screening for drug repositioning against human thymidylate synthase. Journal of Biomolecular Structure and Dynamics, 2022, , 1-17.	3.5	3
13	Rivea hypocrateriformis (Desr.) Choisy: An Overview of Its Ethnomedicinal Uses, Phytochemistry, and Biological Activities and Prospective Research Directions. Journal of Chemistry, 2022, 2022, 1-11.	1.9	3
14	Structural characterization of cassava linamarase-linamarin enzyme complex: an integrated computational approach. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9270-9278.	3.5	2
15	Accommodating receptor flexibility and free energy calculation to reduce false positive binders in the discovery of natural products blockers of SARS-COV-2 spike RBD-ACE2 interface. Biochemistry and Biophysics Reports, 2021, 27, 101024.	1.3	2
16	Conformations and stability of capsaicin in bulk solvents: A molecular dynamics study. Journal of Molecular Liquids, 2022, 345, 117794.	4.9	2
17	A Molecular Investigation of the Solvent Influence on Inter- and Intra-Molecular Hydrogen Bond Interaction of Linamarin. Processes, 2022, 10, 352.	2.8	2
18	Solvent effects on host-guest residence time and kinetics: further insights from metadynamics simulation of Toussaintine-A unbiding from chitosan nanoparticle. Journal of Molecular Modeling, 2021, 27, 127.	1.8	1

#	Article	IF	Citations
19	Abrogating the nsp10â€“nsp16 switching mechanisms in SARS-CoV-2 by phytochemicals from Withania somnifera: a molecular dynamics study. Molecular Simulation, 0, , 1-9.	2.0	1
20	Relaxed complex scheme and molecular dynamics simulation suggests small molecule inhibitor of human TMPRSS2 for combating COVID-19. Journal of Biomolecular Structure and Dynamics, 2021, , 1-11.	3.5	1