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	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
2	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
3	Conformations and stability of capsaicin in bulk solvents: A molecular dynamics study. Journal of Molecular Liquids, 2022, 345, 117794.	4.9	2
4	A Molecular Investigation of the Solvent Influence on Inter- and Intra-Molecular Hydrogen Bond Interaction of Linamarin. Processes, 2022, 10, 352.	2.8	2
5	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
6	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
7	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
8	*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
9	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
10	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
11	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
12	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
13	Cationâ€"Ï€ interactions drive hydrophobic self-assembly and aggregation of niclosamide in water. RSC Advances, 2021, 11, 33136-33147.	3.6	5
14	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
15	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
16	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
17	Solvent effects on molecular encapsulation of Toussantine-A by chitosan nanoparticle: A metadynamics study. Journal of Molecular Liquids, 2019, 292, 111434.	4.9	7
18	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

#	Article	IF	Citations
19	Synthesis of Polyamidoamine Dendrimer for Encapsulating Tetramethylscutellarein for Potential Bioactivity Enhancement. International Journal of Molecular Sciences, 2015, 16, 26363-26377.	4.1	31
20	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