Samantha Weerasinghe

List of Publications by Year
in descending order

20	691	933447 10	794594 19
papers	citations	h-index	g-index

21	21	21	657
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Cracking a cancer code histone deacetylation in epigenetic: the implication from molecular dynamics simulations on efficacy assessment of histone deacetylase inhibitors. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2352-2368.	3.5	11
2	Impact of Cd(II) on the stability of human uracil DNA glycosylase enzyme; an implication of molecular dynamics trajectories on stability analysis. Journal of Biomolecular Structure and Dynamics, 2022, 40, 14027-14034.	3.5	5
3	Implication of Ab Initio, QM/MM, and molecular dynamics calculations on the prediction of the therapeutic potential of some selected HDAC inhibitors. Molecular Simulation, 2022, 48, 1464-1475.	2.0	6
4	Reorientational dynamics of molecules in liquid methane: A molecular dynamics simulation study. Journal of Molecular Liquids, 2021, 324, 114727.	4.9	4
5	Kirkwoodâ€“Buff-Derived Force Field for Peptides and Proteins: Philosophy and Development of KBFF20. Journal of Chemical Theory and Computation, 2021, 17, 2964-2990.	5.3	14
6	Identify the effect of As(III) on the structural stability of monomeric PKM2 and its carcinogenicity: A molecular dynamics and QM/MM based approach. Journal of Molecular Structure, 2021, 1235, 130257.	3.6	8
7	Effects of Hydrogen Bonding on the Rotational Dynamics of Water-Like Molecules in Liquids: Insights from Molecular Dynamics Simulations. Australian Journal of Chemistry, 2020, 73, 734.	0.9	3
8	Plausible compounds drawn from plants as curative agents for neurodegeneration: An in-silico approach. Journal of Computer-Aided Molecular Design, 2020, 34, 1003-1011.	2.9	0
9	Structure and Dynamics of Collagen Hydration Water from Molecular Dynamics Simulations: Implications of Temperature and Pressure. Journal of Physical Chemistry B, 2019, 123, 4901-4914.	2.6	17
10	Exploring the binding properties of agonists interacting with glucocorticoid receptor: an in silico approach. Journal of Molecular Modeling, 2018, 24, 342.	1.8	9
11	Development of an Information System of Structures and Force Field Parameters of Chemical Compounds from Sri Lankan Flora. Combinatorial Chemistry and High Throughput Screening, 2018, 21, 550-556.	1.1	2
12	Rotational-Diffusion Propagator of the Intramolecular Protonâ€“Proton Vector in Liquid Water: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2017, 121, 10893-10905.	2.6	11
13	An In Silico Approach of Coumarin-Derived Inhibitors for Human DNA Topoisomerase I. Australian Journal of Chemistry, 2016, 69, 1005.	0.9	10
14	A Kirkwood-Buff Derived Force Field for Aqueous Alkali Halides. Journal of Chemical Theory and Computation, 2011, 7, 1369-1380.	5.3	128
15	Study of aggregate formation of caffeine in water by molecular dynamics simulation. Computational and Theoretical Chemistry, 2011, 966, 140-148.	2.5	17
16	Development of a molecular mechanics force field for caffeine to investigate the interactions of caffeine in different solvent media. Computational and Theoretical Chemistry, 2010, 944, 116-123.	1.5	18
17	Simulation of structural and functional properties of mevalonate diphosphate decarboxylase (MVD). Journal of Molecular Modeling, 2010, 16, 489-498.	1.8	9
18	Kirkwoodâ€“Buff derived force field for mixtures of acetone and water. Journal of Chemical Physics, 2003, 118, 10663-10670.	3.0	131

#	Article	IF	Citations
19	A Kirkwoodâ^'Buff Derived Force Field for Mixtures of Urea and Water. Journal of Physical Chemistry B, 2003, 107, 3891-3898.	2.6	227
20	Cavity formation and preferential interactions in urea solutions: Dependence on urea aggregation. Journal of Chemical Physics, 2003, 118, 5901-5910.	3.0	46