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	A Kirkwoodâ˜Buff Derived Force Field for Mixtures of Urea and Water. Journal of Physical Chemistry B, 2003, 107, 3891-3898.	2.6	227
2	Kirkwoodâ€“Buff derived force field for mixtures of acetone and water. Journal of Chemical Physics, 2003, 118, 10663-10670.	3.0	131
3	A Kirkwood-Buff Derived Force Field for Aqueous Alkali Halides. Journal of Chemical Theory and Computation, 2011, 7, 1369-1380.	5.3	128
4	Cavity formation and preferential interactions in urea solutions: Dependence on urea aggregation. Journal of Chemical Physics, 2003, 118, 5901-5910.	3.0	46
5	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
6	Study of aggregate formation of caffeine in water by molecular dynamics simulation. Computational and Theoretical Chemistry, 2011, 966, 140-148.	2.5	17
7	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
8	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
9	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
10	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
11	An In Silico Approach of Coumarin-Derived Inhibitors for Human DNA Topoisomerase I. Australian Journal of Chemistry, 2016, 69, 1005.	0.9	10
12	Simulation of structural and functional properties of mevalonate diphosphate decarboxylase (MVD). Journal of Molecular Modeling, 2010, 16, 489-498.	1.8	9
13	Exploring the binding properties of agonists interacting with glucocorticoid receptor: an in silico approach. Journal of Molecular Modeling, 2018, 24, 342.	1.8	9
14	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
15	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
16	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
17	Reorientational dynamics of molecules in liquid methane: A molecular dynamics simulation study. Journal of Molecular Liquids, 2021, 324, 114727.	4.9	4
18	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

#	Article	IF	Citations
19	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
20	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