

Debashree Chakraborty

List of Publications by Year in descending order

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Version: 2024-02-01

31
papers

520
citations

759233

12
h-index

677142

22
g-index

31
all docs

31
docs citations

31
times ranked

553
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular mechanism of inhibition of COVID-19 main protease by $\hat{1}^2$ -adrenoceptor agonists and adenosine deaminase inhibitors using <i>in silico</i> methods. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 5112-5127.	3.5	5
2	Exploring the potential role of quercetin in corrosion inhibition of aluminium alloy 6063 in hydrochloric acid solution by experimental and theoretical studies. <i>Journal of Adhesion Science and Technology</i> , 2022, 36, 2020-2045.	2.6	5
3	Anti-corrosion investigation of a new nitro veratraldehyde substituted imidazopyridine derivative Schiff base on mild steel surface in hydrochloric acid medium: Experimental, computational, surface morphological analysis. <i>Materials Chemistry and Physics</i> , 2022, 281, 125855.	4.0	17
4	Influence of Ion Specificity and Concentration on the Conformational Transition of Intrinsically Disordered Sheep Prion Peptide. <i>ChemPhysChem</i> , 2022, 23, .	2.1	3
5	Exploring the multiple conformational states of RNA genome through interhelical dynamics and network analysis. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108264.	2.4	1
6	Diverse interactions of aggregated insulin with selected coumarin dyes: Time dependent fluorogenicity, simulation studies and comparison with thioflavin T. <i>Dyes and Pigments</i> , 2021, 184, 108796.	3.7	1
7	Structural and dynamical properties of water in surfactant-like peptide-based nanotubes: Effect of pore size, tube length and charge. <i>Journal of Molecular Liquids</i> , 2021, 323, 115033.	4.9	7
8	Theoretical insights into molecular mechanism and energy criteria of PARPase enzyme inhibition by benzimidazole analogues. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 988-1004.	2.6	6
9	Effective inhibition of mild steel corrosion by 6-bromo-(2,4-dimethoxyphenyl)methylidene]imidazo [1,2-a]pyridine-2-carbohydrazide in 0.5M HCl: Insights from experimental and computational study. <i>Journal of Molecular Structure</i> , 2021, 1232, 130074.	3.6	15
10	Temperature-Dependent Conformational Evolution of SARS CoV-2 RNA Genome Using Network Analysis. <i>Journal of Physical Chemistry B</i> , 2021, 125, 10672-10681.	2.6	3
11	Deciphering the competitive inhibition of dihydropteroate synthase by 8 marcaptoguanine analogs: enhanced potency in phenylsulfonyl fragments. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-20.	3.5	3
12	Preferential binding affinity of ions and their effect on structure and dynamics of water near antimicrobial peptide. <i>Journal of Molecular Liquids</i> , 2021, 344, 117789.	4.9	5
13	Effect of hydrophobic and hydrogen bonding interactions on the potency of $\hat{A}^{\hat{Y}}$ alanine analogs of \hat{C} protein coupled glucagon receptor inhibitors. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020, 88, 327-344.	2.6	14
14	Effect of cosolvents in the preferential binding affinity of water in aqueous solutions of amino acids and amides. <i>Journal of Molecular Liquids</i> , 2020, 300, 112375.	4.9	8
15	Epitope-Based Potential Vaccine Candidate for Humoral and Cell-Mediated Immunity to Combat Severe Acute Respiratory Syndrome Coronavirus 2 Pandemic. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 9920-9930.	4.6	12
16	In-silico epitope identification and design of Uricase mutein with reduced immunogenicity. <i>Process Biochemistry</i> , 2020, 92, 288-302.	3.7	6
17	Structural and Thermophysical Anomalies of Liquid Water: A Tale of Molecules in the Instantaneous Low- and High-Density Regions. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1071-1081.	2.6	20
18	Carbohelicenes and thiahelicene from phthalaldehydes through Perkin approach. <i>Journal of Molecular Structure</i> , 2019, 1195, 309-314.	3.6	10

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19	Hydrophilicity of the hydrophobic group: Effect of cosolvents and ions. <i>Journal of Molecular Liquids</i> , 2019, 280, 389-398.	4.9	7
20	Computational insights into factor affecting the potency of diaryl sulfone analogs as <i>Escherichia coli</i> dihydropteroate synthase inhibitors. <i>Computational Biology and Chemistry</i> , 2019, 78, 37-52.	2.3	12
21	Interstitial Voids and Resultant Density of Liquid Water: A First-Principles Molecular Dynamics Study. <i>ACS Omega</i> , 2018, 3, 2010-2017.	3.5	23
22	Stay Wet, Stay Stable? How Internal Water Helps the Stability of Thermophilic Proteins. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12760-12770.	2.6	21
23	Evidence that crystal nucleation in aqueous NaCl solution Occurs by the two-step mechanism. <i>Chemical Physics Letters</i> , 2013, 587, 25-29.	2.6	53
24	How Crystals Nucleate and Grow in Aqueous NaCl Solution. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 573-578.	4.6	85
25	A first principles simulation study of fluctuations of hydrogen bonds and vibrational frequencies of water at liquid-vapor interface. <i>Chemical Physics</i> , 2012, 392, 96-104.	1.9	39
26	Voids and necks in liquid ammonia and their roles in diffusion of ions of varying size. <i>Journal of Computational Chemistry</i> , 2012, 33, 843-852.	3.3	8
27	An analysis of voids and necks in supercritical water. <i>Journal of Molecular Liquids</i> , 2011, 163, 1-6.	4.9	24
28	Diffusion of ions in supercritical water: Dependence on ion size and solvent density and roles of voids and necks. <i>Journal of Molecular Liquids</i> , 2011, 162, 12-19.	4.9	19
29	Hydrogen bonded structure and dynamics of liquid-vapor interface of water-ammonia mixture: An <i>ab initio</i> molecular dynamics study. <i>Journal of Chemical Physics</i> , 2011, 135, 114510.	3.0	38
30	Pressure effects on diffusion in liquid ammonia : A simulation study using a combination of isobaric-isothermal and microcanonical molecular dynamics. <i>Indian Journal of Physics</i> , 2009, 83, 91-100.	1.8	11
31	Effects of ion concentration on the hydrogen bonded structure of water in the vicinity of ions in aqueous NaCl solutions. <i>Journal of Chemical Sciences</i> , 2008, 120, 71-77.	1.5	39