Syed Tarique Moin

List of Publications by Year
in descending order

38	618	687363 13	610901 24
papers	citations	h-index	g-index

38	38	38	947
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hydration modulates oxygen channel residues for oxygenation of cysteine dioxygenase: Perspectives from molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2022, 110, 108060.	2.4	1
2	Investigation of the structural and dynamical properties of human uncoupling protein 2 through molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2022, 114, 108203.	2.4	2
3	Dynamics of metal binding and mutation in yybPâ€“ykoY riboswitch of Lactococcus lactis. RSC Advances, 2022, 12, 17337-17349.	3.6	0
4	Interaction of Phthalates with Lipid Bilayer Membranes. Journal of Physical Chemistry B, 2022, 126, 4679-4688.	2.6	3
5	Evaluation of a sesquiterpene as possible drug lead against gelatinases via molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1645-1660.	3.5	4
6	Exploring interfacial dynamics in homodimeric S-ribosylhomocysteine lyase (LuxS) from Vibrio cholerae through molecular dynamics simulations. RSC Advances, 2021, 11, 1700-1714.	3.6	2
7	Dynamic Profiling of Î²-Coronavirus 3CL M^{pro} Protease Ligand-Binding Sites. Journal of Chemical Information and Modeling, 2021, 61, 3058-3073.	5.4	35
8	Iron coordination to pyochelin siderophore influences dynamics of FptA receptor from Pseudomonas aeruginosa: a molecular dynamics simulation study. BioMetals, 2021, 34, 1099-1119.	4.1	2
9	Inter-Subunit Dynamics Controls Tunnel Formation During the Oxygenation Process in Hemocyanin Hexamers. Frontiers in Molecular Biosciences, 2021, 8, 710623.	3.5	4
10	Editorial: Molecular Dynamics Simulations of Metalloproteins and Metalloenzymes. Frontiers in Chemistry, 2021, 9, 789299.	3.6	1
11	Solvation of cholesterol in different solvents: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2020, 22, 1154-1167.	2.8	16
12	Piperidiniumâ€Based Deep Eutectic Solvents: Efficient and Sustainable Ecoâ€Friendly Medium for Oneâ€Pot Nâ€Heterocycles Synthesis. ChemistrySelect, 2020, 5, 12697-12703.	1.5	3
13	Carbazoleâ€Linked 1,2,3â€Triazoles: In Vitro Î² â€Glucuronidase Inhibitory Potential, Kinetics, and Molecular Docking Studies. ChemistrySelect, 2019, 4, 6181-6189.	1.5	3
14	Highly selective enrichment of phosphopeptides using poly(dibenzoâ€18â€crownâ€6) as a solidâ€phase extraction material. Biomedical Chromatography, 2019, 33, e4567.	1.7	2
15	Hydration of Closely Related Manganese and Magnesium Porphyrins in Aqueous Solutions: Ab Initio Quantum Mechanical Charge Field Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2019, 123, 10769-10779.	2.6	3
16	Understanding LuxS-based quorum sensing and its inhibition â€“ molecular dynamics simulation study. Molecular Simulation, 2018, 44, 558-567.	2.0	2
17	Morpholinium and Piperidinium Based Deep Eutectic Solvents for Synthesis of Pyrazoleâ€5â€Carbonitriles, Indoles and Tetrazoles: Bulk Properties via Molecular Dynamics Simulations. ChemistrySelect, 2018, 3, 12907-12917.	1.5	10
18	Hydration facilitates oxygenation of hemocyanin: perspectives from molecular dynamics simulations. European Biophysics Journal, 2018, 47, 925-938.	2.2	2

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19	Identification of Histone Deacetylase (HDAC) as a drug target against MRSA via interolog method of protein-protein interaction prediction. European Journal of Pharmaceutical Sciences, 2017, 106, 198-211.	4.0	8
20	Syntheses of 4,6-dihydroxypyrimidine diones, their urease inhibition, in vitro, in silico, and kinetic studies. Bioorganic Chemistry, 2017, 75, 317-331.	4.1	12
21	Hydration of ironâ€“porphyrins: ab initio quantum mechanical charge field molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2017, 19, 30822-30833.	2.8	3
22	N,N-Dimethylpyridin-4-amine (DMAP) based ionic liquids: evaluation of physical properties via molecular dynamics simulations and application as a catalyst for Fisher indole and 1H-tetrazole synthesis. RSC Advances, 2017, 7, 34197-34207.	3.6	14
23	Active site characterization and structure based 3D-QSAR studies on non-redox type 5-lipoxygenase inhibitors. European Journal of Pharmaceutical Sciences, 2016, 88, 26-36.	4.0	9
24	Zinc- and copper-porphyrins in aqueous solution â€“ two similar complexes with strongly contrasting hydration. Molecular BioSystems, 2016, 12, 2288-2295.	2.9	6
25	Synthesis and in vitro Î±-chymotrypsin inhibitory activity of 6-chlorobenzimidazole derivatives. Bioorganic and Medicinal Chemistry, 2016, 24, 3387-3395.	3.0	12
26	Solvent-free 1H-tetrazole, 1,2,5,6-tetrahydronicotinonitrile and pyrazole synthesis using quinoline based ionic fluoride salts (QuFs): thermal and theoretical studies. RSC Advances, 2015, 5, 95061-95072.	3.6	7
27	2-Arylquinazolin-4(3H)-ones: A new class of Î±-glucosidase inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 7417-7421.	3.0	51
28	Hydration of the cyanide ion: an ab initio quantum mechanical charge field molecular dynamics study. Physical Chemistry Chemical Physics, 2014, 16, 26075-26083.	2.8	4
29	Solvent-free click chemistry for tetrazole synthesis from 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-Based fluorinated ionic liquids, their micellization, and density functional theory studies. RSC Advances, 2014, 4, 64128-64137.	3.6	20
30	Hydration of porphyrin and Mgâ€“porphyrin: ab initio quantum mechanical charge field molecular dynamics simulations. Molecular BioSystems, 2014, 10, 117-127.	2.9	15
31	Dynamics of ligand exchange mechanism at Cu(II) in water: An ab initio quantum mechanical charge field molecular dynamics study with extended quantum mechanical region. Journal of Chemical Physics, 2013, 139, 014503.	3.0	25
32	Activation of TrkB receptors by NGFÎ² mimetic peptide conjugated polymersome nanoparticles. Nanomedicine: Nanotechnology, Biology, and Medicine, 2012, 8, 271-274.	3.3	20
33	Sulfur Dioxide in Water: Structure and Dynamics Studied by an Ab Initio Quantum Mechanical Charge Field Molecular Dynamics Simulation. Inorganic Chemistry, 2011, 50, 3379-3386.	4.0	15
34	Molecular dynamics simulation of mammalian 15S-lipoxygenase with AMBER force field. European Biophysics Journal, 2011, 40, 715-726.	2.2	18
35	Carbon dioxide in aqueous environmentâ€"A quantum mechanical charge field molecular dynamics study. International Journal of Quantum Chemistry, 2011, 111, 1370-1378.	2.0	13
36	Structure and dynamics of methanol in water: A quantum mechanical charge field molecular dynamics study. Journal of Computational Chemistry, 2011, 32, 886-892.	3.3	11

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37	A Quantum Mechanical Charge Field Molecular Dynamics Study of Fe²⁺ and Fe³⁺ Ions in Aqueous Solutions. Inorganic Chemistry, 2010, 49, 5101-5106.	4.0	48
38	Analgesic and Antioxidant Activity of Mangiferin and Its Derivatives: the Structure Activity Relationship. Biological and Pharmaceutical Bulletin, 2005, 28, 596-600.	1.4	212