Tusar Bandyopadhyay

List of Publications by Year
in descending order

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35	380	686830	839053
papers	citations	13 h-index	18 g-index

37	37	37	426
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Unbinding of hACE2 and inhibitors from the receptor binding domain of SARS-CoV-2 spike protein. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3245-3264.	2.0	2
2	MD simulation reveals differential binding of Cm(III) and Th(IV) with serum transferrin at acidic pH. Proteins: Structure, Function and Bioinformatics, 2021, 89, 193-206.	1.5	4
3	Heat-induced transitions of an empty minute virus of mice capsid in explicit water: all-atom MD simulation. Journal of Biomolecular Structure and Dynamics, 2021, , 1-14.	2.0	1
4	Quantum chemical and well-tempered metadynamics study to design adenine analogs for orthogonal Preq1 riboswitch. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4635-4643.	2.0	0
5	Molecular dynamics simulations of plutonium binding and its decorporation from the binding-cleft of human serum transferrin. Journal of Biological Inorganic Chemistry, 2020, 25, 213-231.	1.1	5
6	Probing the Role of Imidazopyridine and Imidazophosphorine Scaffolds To Design Novel Proton Pump Inhibitor for H+,K+-ATPase: A DFT Study. ACS Omega, 2019, 4, 1311-1321.	1.6	0
7	Temperature Induced Dynamical Transition of Biomolecules in Polarizable and Nonpolarizable TIP3P Water. Journal of Chemical Theory and Computation, 2019, 15, 2706-2718.	2.3	8
8	Binding of Cm(III) and Th(IV) with Human Transferrin at Serum pH: Combined QM and MD Investigations. Journal of Physical Chemistry B, 2019, 123, 2729-2744.	1.2	7
9	Dynamic Mechanism of a Fluorinated Oxime Reactivator Unbinding from AChE Gorge in Polarizable Water. Journal of Physical Chemistry B, 2018, 122, 3876-3888.	1.2	9
10	Stereoselective Metabolism of Omeprazole by Cytochrome P450 2C19 and 3A4: Mechanistic Insights from DFT Study. Journal of Physical Chemistry B, 2018, 122, 5765-5775.	1.2	16
11	Unbinding of fluorinated oxime drug from the AChE gorge in polarizable water: a well-tempered metadynamics study. Physical Chemistry Chemical Physics, 2017, 19, 5560-5569.	1.3	13
12	Water isotope effect on the thermostability of a polio viral RNA hairpin: A metadynamics study. Journal of Chemical Physics, 2017, 146, 165104.	1.2	17
13	Divalent ions are potential permeating blockers of the non-selective NaK ion channel: combined QM and MD based investigations. Physical Chemistry Chemical Physics, 2017, 19, 27611-27622.	1.3	7
14	Designed inhibitors with hetero linkers for gastric proton pump H + ,K + -ATPase: Steered molecular dynamics and metadynamics studies. Journal of Molecular Graphics and Modelling, 2017, 78, 129-138.	1.3	2
15	Selective separation of strontium by multitopic ionâ€pair receptor: A DFT exploration. International Journal of Quantum Chemistry, 2017, 117, e25418.	1.0	6
16	Revealing the Mechanistic Pathway of Acid Activation of Proton Pump Inhibitors To Inhibit the Gastric Proton Pump: A DFT Study. Journal of Physical Chemistry B, 2016, 120, 13031-13038.	1.2	18
17	Role of Noncovalent Interactions in Designing Inhibitors for H⁺,K⁺â€ATPase: Combined QM and MD Based Investigations. ChemistrySelect, 2016, 1, 6847-6854.	0.7	3
18	Solvation of arsenate anion: combined quantum mechanics and molecular dynamics based investigation. Molecular Physics, 2016, 114, 2029-2036.	0.8	3

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19	Orthoâ€7 bound to the activeâ€site gorge of free and <scp>OP</scp>â€conjugated acetylcholinesterase: Cationâ€Î€ interactions. Biopolymers, 2016, 105, 10-20.	1.2	5
20	Efficient Separation of Europium Over Americium Using Cucurbit-[5]-uril Supramolecule: A Relativistic DFT Based Investigation. Inorganic Chemistry, 2016, 55, 598-609.	1.9	38
21	Selectivity of a Singly Permeating Ion in Nonselective NaK Channel: Combined QM and MD Based Investigations. Journal of Physical Chemistry B, 2015, 119, 12783-12797.	1.2	18
22	Proteinâ€“Drug Interactions with Effective Polarization in Polarizable Water: Oxime Unbinding from AChE Gorge. Journal of Physical Chemistry B, 2015, 119, 14460-14471.	1.2	23
23	Water-Mediated Differential Binding of Strontium and Cesium Cations in Fulvic Acid. Journal of Physical Chemistry B, 2015, 119, 10989-10997.	1.2	20
24	Unbinding free energy of acetylcholinesterase bound oxime drugs along the gorge pathway from metadynamics-umbrella sampling investigation. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1799-1818.	1.5	16
25	Energetics of Ortho-7 (Oxime Drug) Translocation through the Active-Site Gorge of Tabun Conjugated Acetylcholinesterase. PLoS ONE, 2012, 7, e40188.	1.1	11
26	Can Functionalized Cucurbituril Bind Actinyl Cations Efficiently? A Density Functional Theory Based Investigation. Journal of Physical Chemistry A, 2012, 116, 4388-4395.	1.1	50
27	Probing O-dealkylation and deamination aging processes in tabun-conjugated AChE: a computational study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	2
28	Solvolysis process of organophosphorus compound P-[2-(dimethylamino)ethyl]-N,N-dimethylphosphonamidic fluoride with simple and Î±-nucleophiles: a DFT study. Theoretical Chemistry Accounts, 2010, 127, 39-47.	0.5	13
29	Differential binding of bispyridinium oxime drugs with acetylcholinesterase. Acta Pharmacologica Sinica, 2010, 31, 313-328.	2.8	18
30	Single-file diffusion through inhomogeneous nanopores. Journal of Chemical Physics, 2008, 128, 114712.	1.2	7
31	Bursts in single-file motion mediated conduction. Journal of Chemical Physics, 2006, 125, 201103.	1.2	7
32	Diffusion-Influenced Fluorescence Quenching by Electron Transfer: The Effect of an External Electric Field. Israel Journal of Chemistry, 2004, 44, 119-125.	1.0	1
33	Coherent and incoherent trapping of a diffusion-assisted system in the presence of an external periodic field. Physical Review E, 2003, 67, 061113.	0.8	0
34	Diffusion assisted endâ€“toâ€“end relaxation of a flexible Rouse polymer chain: Fluorescence quenching through a model energy transfer. Journal of Chemical Physics, 2003, 119, 572-584.	1.2	13
35	Diffusion influenced end-to-end reaction of a flexible polymer chain: The memory effect. Journal of Chemical Physics, 2002, 116, 4366-4369.	1.2	17