

Kalyanashis Jana

List of Publications by Year in descending order

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papers

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758635

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459
citing authors

#	ARTICLE	IF	CITATIONS
1	Revealing the cholinergic inhibition mechanism of Alzheimer's by galantamine: a metadynamics simulation study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 5100-5111.	2.0	11
2	The mechanism of conversion of substituted glycals to chiral acenes via Diels-Alder reaction: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 6353-6367.	1.5	1
3	Structural insights into the interactions of flavin mononucleotide (FMN) and riboflavin with FMN riboswitch: a molecular dynamics simulation study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 3856-3866.	2.0	3
4	Quantum chemical and well-tempered metadynamics study to design adenine analogs for orthogonal Preq1 riboswitch. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 4635-4643.	2.0	0
5	Common mechanism of thermostability in small α - and β -proteins studied by molecular dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020, 88, 1233-1250.	1.5	4
6	Flexible Fitting of Small Molecules into Electron Microscopy Maps Using Molecular Dynamics Simulations with Neural Network Potentials. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2591-2604.	2.5	24
7	Probing the Role of Imidazopyridine and Imidazophosphorine Scaffolds To Design Novel Proton Pump Inhibitor for H ⁺ ,K ⁺ -ATPase: A DFT Study. <i>ACS Omega</i> , 2019, 4, 1311-1321.	1.6	0
8	Revealing the mechanistic pathway of cholinergic inhibition of Alzheimer's disease by donepezil: a metadynamics simulation study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13578-13589.	1.3	20
9	Indium-Catalyzed Denitrogenative Transannulation of Pyridotriazoles: Synthesis of Pyrido[1,2- <i>a</i>]indoles. <i>Organic Letters</i> , 2019, 21, 2043-2047.	2.4	35
10	Transformation of Substituted Glycals to Chiral Fused Aromatic Cores via Annulative β -Extension Reactions with Arynes. <i>Organic Letters</i> , 2018, 20, 1572-1575.	2.4	17
11	DFT studies on quantum mechanical tunneling in tautomerization of three-membered rings. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28049-28058.	1.3	8
12	Probing the Structural and Electronic Effects on the Origin of β -Facial Stereoselectivity in 1-Methylphosphole 1-Oxide Cycloadditions and Cyclodimerization. <i>ACS Omega</i> , 2018, 3, 10945-10952.	1.6	2
13	Instant Detection of Hydrogen Cyanide Gas and Cyanide Salts in Solid Matrices and Water by using Cu ^{II} and Ni ^{II} Complexes of Intramolecularly Hydrogen Bonded Zwitterions. <i>Chemistry - A European Journal</i> , 2018, 24, 10721-10731.	1.7	12
14	Stereoselective Metabolism of Omeprazole by Cytochrome P450 2C19 and 3A4: Mechanistic Insights from DFT Study. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5765-5775.	1.2	16
15	DFT Study To Explore the Importance of Ring Size and Effect of Solvents on the Keto-Enol Tautomerization Process of β - and γ -Cyclodiones. <i>ACS Omega</i> , 2018, 3, 8429-8439.	1.6	23
16	Influence of gauche effect on uncharged oxime reactivators for the reactivation of tabun-inhibited AChE: quantum chemical and steered molecular dynamics studies. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 793-807.	1.3	4
17	Designed inhibitors with hetero linkers for gastric proton pump H ⁺ ,K ⁺ -ATPase: Steered molecular dynamics and metadynamics studies. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 78, 129-138.	1.3	2
18	The role of non-covalent interaction for the adsorption of CO ₂ and hydrocarbons with per-hydroxylated pillar[6]arene: a computational study. <i>New Journal of Chemistry</i> , 2017, 41, 12044-12051.	1.4	32

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19	Nitrene insertion into an adjacent o -methoxy group followed by nucleophilic addition to the heterocumulene intermediate: Experimental and computational studies. <i>Tetrahedron</i> , 2017, 73, 5280-5288.	1.0	5
20	Revealing the importance of linkers in K-series oxime reactivators for tabun-inhibited AChE using quantum chemical, docking and SMD studies. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 729-742.	1.3	7
21	Improved Shoot Regeneration, Salinity Tolerance and Reduced Fungal Susceptibility in Transgenic Tobacco Constitutively Expressing PR-10a Gene. <i>Frontiers in Plant Science</i> , 2016, 7, 217.	1.7	22
22	Revealing the Mechanistic Pathway of Acid Activation of Proton Pump Inhibitors To Inhibit the Gastric Proton Pump: A DFT Study. <i>Journal of Physical Chemistry B</i> , 2016, 120, 13031-13038.	1.2	18
23	Role of Noncovalent Interactions in Designing Inhibitors for H ⁺ ,K ⁺ -ATPase: Combined QM and MD Based Investigations. <i>ChemistrySelect</i> , 2016, 1, 6847-6854.	0.7	3
24	In silico studies with substituted adenines to achieve a remarkable stability of mispairs with thymine nucleobase. <i>New Journal of Chemistry</i> , 2016, 40, 1807-1816.	1.4	8
25	Asymmetric Henry reaction of trifluoromethyl ketone and aldehyde using Cu(II)-complex: computational study offers the origin of enantioselectivity with varied size of catalysts. <i>Tetrahedron</i> , 2015, 71, 5229-5237.	1.0	28
26	In Silico Studies to Explore the Mutagenic Ability of 5-Halo/Oxy/Li-Oxy-Uracil Bases with Guanine of DNA Base Pairs. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9753-9761.	1.1	13
27	Hydrogen Bonding Interaction between Active Methylene Hydrogen Atoms and an Anion as a Binding Motif for Anion Recognition: Experimental Studies and Theoretical Rationalization. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2656-2666.	1.1	9