Kalyanashis Jana

List of Publications by Year
in descending order

27	330	758635	887659
papers	citations	12 h-index	17 g-index

29	29	29	459
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Indium-Catalyzed Denitrogenative Transannulation of Pyridotriazoles: Synthesis of Pyrido[1,2-a]indoles. Organic Letters, 2019, 21, 2043-2047.	2.4	35
2	The role of non-covalent interaction for the adsorption of CO₂ and hydrocarbons with per-hydroxylated pillar[6]arene: a computational study. New Journal of Chemistry, 2017, 41, 12044-12051.	1.4	32
3	Asymmetric Henry reaction of trifluoromethyl ketone and aldehyde using Cu(II)-complex: computational study offers the origin of enantioselectivity with varied size of catalysts. Tetrahedron, 2015, 71, 5229-5237.	1.0	28
4	Flexible Fitting of Small Molecules into Electron Microscopy Maps Using Molecular Dynamics Simulations with Neural Network Potentials. Journal of Chemical Information and Modeling, 2020, 60, 2591-2604.	2.5	24
5	DFT Study To Explore the Importance of Ring Size and Effect of Solvents on the Ketoâ€“Enol Tautomerization Process of Î±- and Î²-Cyclodiones. ACS Omega, 2018, 3, 8429-8439.	1.6	23
6	Improved Shoot Regeneration, Salinity Tolerance and Reduced Fungal Susceptibility in Transgenic Tobacco Constitutively Expressing PR-10a Gene. Frontiers in Plant Science, 2016, 7, 217.	1.7	22
7	Revealing the mechanistic pathway of cholinergic inhibition of Alzheimer's disease by donepezil: a metadynamics simulation study. Physical Chemistry Chemical Physics, 2019, 21, 13578-13589.	1.3	20
8	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
9	Transformation of Substituted Glycals to Chiral Fused Aromatic Cores via Annulative Ï€-Extension Reactions with Arynes. Organic Letters, 2018, 20, 1572-1575.	2.4	17
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	In Silico Studies to Explore the Mutagenic Ability of 5-Halo/Oxy/Li-Oxy-Uracil Bases with Guanine of DNA Base Pairs. Journal of Physical Chemistry A, 2014, 118, 9753-9761.	1.1	13
12	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. Chemistry - A European Journal, 2018, 24, 10721-10731.	1.7	12
13	Revealing the cholinergic inhibition mechanism of Alzheimerâ€™s by galantamine: a metadynamics simulation study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5100-5111.	2.0	11
14	Hydrogen Bonding Interaction between Active Methylene Hydrogen Atoms and an Anion as a Binding Motif for Anion Recognition: Experimental Studies and Theoretical Rationalization. Journal of Physical Chemistry A, 2014, 118, 2656-2666.	1.1	9
15	In silico studies with substituted adenines to achieve a remarkable stability of mispairs with thymine nucleobase. New Journal of Chemistry, 2016, 40, 1807-1816.	1.4	8
16	DFT studies on quantum mechanical tunneling in tautomerization of three-membered rings. Physical Chemistry Chemical Physics, 2018, 20, 28049-28058.	1.3	8
17	Revealing the importance of linkers in K-series oxime reactivators for tabun-inhibited AChE using quantum chemical, docking and SMD studies. Journal of Computer-Aided Molecular Design, 2017, 31, 729-742.	1.3	7
18	Nitrene insertion into an adjacent o -methoxy group followed by nucleophilic addition to the heterocumulene intermediate: Experimental and computational studies. Tetrahedron, 2017, 73, 5280-5288.	1.0	5

#	Article	IF	Citations
19	Influence of gauche effect on uncharged oxime reactivators for the reactivation of tabun-inhibited AChE: quantum chemical and steered molecular dynamics studies. Journal of Computer-Aided Molecular Design, 2018, 32, 793-807.	1.3	4
20	Common mechanism of thermostability in small Î±â€•and Î²â€proteins studied by molecular dynamics. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1233-1250.	1.5	4
21	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
22	Structural insights into the interactions of flavin mononucleotide (FMN) and riboflavin with FMN riboswitch: a molecular dynamics simulation study. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3856-3866.	2.0	3
23	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
24	Probing the Structural and Electronic Effects on the Origin of Ï€-Facial Stereoselectivity in 1-Methylphosphole 1-Oxide Cycloadditions and Cyclodimerization. ACS Omega, 2018, 3, 10945-10952.	1.6	2
25	The mechanism of conversion of substituted glycals to chiral acenes via Dielsâ€“Alder reaction: a computational study. Organic and Biomolecular Chemistry, 2021, 19, 6353-6367.	1.5	1
26	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
27	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