Raman Kumar Singh

List of Publications by Year
in descending order

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11 papers	203 citations	1307594 7 h-index	1281871 11 g-index
11 all docs	11 docs citations	11 times ranked	332 citing authors

#	Article	IF	Citations
1	Synthesis of Antibacterial Disulfide Derivatives and its Computational Molecular Docking Against Penicillin Binding Protein. Analytical Chemistry Letters, 2021, 11, 618-634.	1.0	3
2	Hydration, Prediction of the pK_a, and Infrared Spectroscopic Study of Sulfonated Polybenzophenone (SPK) Block-Copolymer Hydrocarbon Membranes and Comparisons with Nafion. ACS Omega, 2021, 6, 32739-32748.	3.5	7
3	Copper(II) and Nickel(II) Complexes of Tridentate Hydrazide and Schiff Base Ligands Containing Phenyl and Naphthalyl Groups: Synthesis, Structural, Molecular Docking and Density Functional Study. Journal of Inorganic and Organometallic Polymers and Materials, 2020, 30, 4426-4440.	3.7	12
4	Diagrams for comprehensive molecular orbital-based chemical reaction analyses: reactive orbital energy diagrams. Physical Chemistry Chemical Physics, 2018, 20, 14211-14222.	2.8	8
5	Theoretical Investigation of the H₂O₂-Induced Degradation Mechanism of Hydrated Nafion Membrane via Ether-Linkage Dissociation. ACS Omega, 2017, 2, 4053-4064.	3.5	29
6	On lowâ€lying excited states of extended nanographenes. Journal of Computational Chemistry, 2017, 38, 2020-2029.	3.3	15
7	Orbital Energy-Based Reaction Analysis of SN2 Reactions. Computation, 2016, 4, 23.	2.0	5
8	Relationship between orbital energy gaps and excitation energies for longâ€chain systems. Journal of Computational Chemistry, 2016, 37, 1451-1462.	3.3	15
9	Experimental and Theoretical Infrared Spectroscopic Study on Hydrated Nafion Membrane. Macromolecules, 2016, 49, 6621-6629.	4.8	58
10	Reactivity index based on orbital energies. Journal of Computational Chemistry, 2014, 35, 1093-1100.	3.3	18
11	Reaction energetics on longâ€range corrected density functional theory: Dielsâ€“Alder reactions. Journal of Computational Chemistry, 2013, 34, 379-386.	3.3	33