

Nabajyoti Baildya

List of Publications by Year in descending order

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Version: 2024-02-01

24
papers

311
citations

1040056
9
h-index

888059
17
g-index

24
all docs

24
docs citations

24
times ranked

280
citing authors

#	ARTICLE	IF	CITATIONS
1	Screening of potential drug from <i>Azadirachta Indica</i> (Neem) extracts for SARS-CoV-2: An insight from molecular docking and MD-simulation studies. <i>Journal of Molecular Structure</i> , 2021, 1227, 129390.	3.6	78
2	Inhibitory activity of hydroxychloroquine on COVID-19 main protease: An insight from MD-simulation studies. <i>Journal of Molecular Structure</i> , 2020, 1219, 128595.	3.6	64
3	Inhibitory efficiency of potential drugs against SARS-CoV-2 by blocking human angiotensin converting enzyme-2: Virtual screening and molecular dynamics study. <i>Microbial Pathogenesis</i> , 2021, 152, 104762.	2.9	23
4	Inhibitory efficacy of RNA virus drugs against SARS-CoV-2 proteins: An extensive study. <i>Journal of Molecular Structure</i> , 2021, 1234, 130152.	3.6	19
5	Inhibitory capacity of chloroquine against SARS-COV-2 by effective binding with angiotensin converting enzyme-2 receptor: An insight from molecular docking and MD-simulation studies. <i>Journal of Molecular Structure</i> , 2021, 1230, 129891.	3.6	18
6	Inhibitory effect of anti-HIV compounds extracted from Indian medicinal plants to retard the replication and transcription process of SARS-CoV-2: an insight from molecular docking and MD-simulation studies. <i>Network Modeling Analysis in Health Informatics and Bioinformatics</i> , 2021, 10, 32.	2.1	16
7	Dehydroabietylamine-decorated imino-phenols: supramolecular gelation and gel phase selective detection of Fe^{3+} , Cu^{2+} and Hg^{2+} ions under different experimental conditions. <i>New Journal of Chemistry</i> , 2022, 46, 8817-8826.	2.8	14
8	A new 1,2,3-triazole-decorated imino-phenol: selective sensing of Zn^{2+} , Cu^{2+} and picric acid under different experimental conditions. <i>New Journal of Chemistry</i> , 2021, 45, 10923-10929.	2.8	12
9	Yttrium nitrate catalyzed synthesis, photophysical study, and TD-DFT calculation of 2,3-dihydroquinazolin-4(1H)-ones. <i>Heteroatom Chemistry</i> , 2017, 28, .	0.7	11
10	Naphthalimide-decorated imino-phenol: supramolecular gelation and selective sensing of Fe^{3+} and Cu^{2+} ions under different experimental conditions. <i>New Journal of Chemistry</i> , 2021, 45, 5213-5220.	2.8	8
11	Environmentally hazardous gas sensing ability of MoS_2 -nanotubes: an insight from the electronic structure and transport properties. <i>Nanoscale Advances</i> , 2021, 3, 4528-4535.	4.6	7
12	Screening of potential anti-HIV compounds from <i>Achyranthes aspera</i> extracts for SARS-CoV-2: An insight from molecular docking study. <i>Journal of Physics: Conference Series</i> , 2021, 1797, 012042.	0.4	6
13	Anti-corrosive properties of quercetin and its derivatives on Fe(111) surface: a quantum chemical approach. <i>SN Applied Sciences</i> , 2019, 1, 1.	2.9	5
14	CO ₂ activation on transition metal decorated graphene quantum dots: An insight from first principles. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 135, 114993.	2.7	5
15	Comparative study of CO ₂ activation on alkali metals encapsulated III-V hollow nanocages: An insight from first-principles calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2021, 412, 127554.	2.1	4
16	Synthesis, photocatalytic and antibacterial activities of a PDS-activated MgO nanocatalyst: experimental and theoretical studies. <i>New Journal of Chemistry</i> , 2022, 46, 6694-6707.	2.8	4
17	Tailoring electronic and transport properties of edge-terminated armchair graphene by defect formation and N/B doping. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126194.	2.1	3
18	Anti-enteric efficacy and mode of action of tridecanoic acid methyl ester isolated from <i>Monochoria hastata</i> (L.) Solms leaf. <i>Brazilian Journal of Microbiology</i> , 2022, , 1.	2.0	3

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19	Repurposing of anti-lung cancer drugs as multi-target inhibitors of SARS-CoV-2 proteins: An insight from molecular docking and MD-simulation study. Microbial Pathogenesis, 2022, 169, 105615.	2.9	3
20	Interaction of copper nanoparticles with DNA: structural and docking studies. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1256-1261.	3.5	2
21	Dipyromethane-Based Receptor for Fluorometric Sensing of Hydrogenpyrophosphate. ChemistrySelect, 2021, 6, 8932-8937.	1.5	2
22	Silver-Ion-Selective Gelation of Simple Pyridine-Naphthalimide Conjugates with Multiple Applications: Sensing, Drug Delivery, Dye Adsorption and Ion Conductivity. ChemistrySelect, 2021, 6, 11696-11705.	1.5	2
23	Inhibitory effect of compounds extracted from Monochoria hastata (L.) Solms on SARS-CoV-2 main protease: An insight from molecular docking and MD-simulation studies. Journal of Molecular Structure, 2022, 1257, 132644.	3.6	2
24	Adenyl nitro urea in molecular recognition of fluoride and pyruvate. Canadian Journal of Chemistry, 2021, 99, 1000000.	1.1	0