Arun Bahadur Gurung

List of Publications by Year
in descending order

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43 papers	645 citations	758635 12 h-index	610482 24 g-index
43 all docs	43 docs citations	43 times ranked	967 citing authors

#	Article	IF	Citations
1	Molecular modelling studies unveil potential binding sites on human serum albumin for selected experimental and in silico COVID-19 drug candidate molecules. Saudi Journal of Biological Sciences, 2022, 29, 53-64.	1.8	10
2	In silico analyses of major active constituents of fingerroot (Boesenbergia rotunda) unveils inhibitory activities against SARS-CoV-2 main protease enzyme. Saudi Journal of Biological Sciences, 2022, 29, 65-74.	1.8	14
3	Insights into plastome of Fagonia indica Burm.f. (Zygophyllaceae): organization, annotation and phylogeny. Saudi Journal of Biological Sciences, 2022, 29, 1313-1321.	1.8	0
4	Artesunate induces substantial topological alterations in the SARS-CoV-2 Nsp1 protein structure. Journal of King Saud University - Science, 2022, 34, 101810.	1.6	8
5	Structural and functional insights into the major mutations of SARS-CoV-2 Spike RBD and its interaction with human ACE2 receptor. Journal of King Saud University - Science, 2022, 34, 101773.	1.6	9
6	RNA-Seq analysis reveals the role of MYB12, MYB111 and MBW complex repressors in regulation of flavonoid biosynthesis in stigmas of saffron (Crocus sativus L.) flowers. Acta Physiologiae Plantarum, 2022, 44, 1.	1.0	4
7	Transcriptome characterization of Larrea tridentata and identification of genes associated with phenylpropanoid metabolic pathways. PLoS ONE, 2022, 17, e0265231.	1.1	1
8	An in silico approach unveils the potential of antiviral compounds in preclinical and clinical trials as SARS-CoV-2 omicron inhibitors. Saudi Journal of Biological Sciences, 2022, 29, 103297.	1.8	11
9	Potential of antiviral peptide-based SARS-CoV-2 inactivators to combat COVID-19. PLoS ONE, 2022, 17, e0268919.	1.1	2
10	The potential of Paritaprevir and Emetine as inhibitors of SARS-CoV-2 RdRp. Saudi Journal of Biological Sciences, 2021, 28, 1426-1432.	1.8	11
11	Identification of potential SARS-CoV-2 entry inhibitors by targeting the interface region between the spike RBD and human ACE2. Journal of Infection and Public Health, 2021, 14, 227-237.	1.9	11
12	Plastome of Saraca asoca (Detarioideae, Fabaceae): Annotation, comparison among subfamily and molecular typing. Saudi Journal of Biological Sciences, 2021, 28, 1487-1493.	1.8	5
13	Identification of novel drug candidates for the inhibition of catalytic cleavage activity of coronavirus 3CL-like protease enzyme. Current Pharmaceutical Biotechnology, 2021, 22, .	0.9	1
14	An Updated Review of Computer-Aided Drug Design and Its Application to COVID-19. BioMed Research International, 2021, 2021, 1-18.	0.9	95
15	The cp genome characterization of Adenium obesum: Gene content, repeat organization and phylogeny. Saudi Journal of Biological Sciences, 2021, 28, 3768-3775.	1.8	4
16	Molecular docking and dynamics simulation study of bioactive compounds from Ficus carica L. with important anticancer drug targets. PLoS ONE, 2021, 16, e0254035.	1.1	32
17	Identification of SARS-CoV-2 inhibitors from extracts of Houttuynia cordata Thunb.. Saudi Journal of Biological Sciences, 2021, 28, 7517-7527.	1.8	13
18	Data-mining technique identifies potential target proteins playing a dual role in inflammation and oxidative stress pathways in relation to atherosclerosis plaque development. Informatics in Medicine Unlocked, 2020, 18, 100278.	1.9	1

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19	Identification of potential drug-like molecules for inhibition of the inflammatory activity of cyclooxygenase-2. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5293-5306.	2.0	1
20	In silico molecular modelling, structural dynamics simulation and characterization of antifungal nature of Î²-glucosidase enzyme from Sechium edule. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-9.	2.0	3
21	Structure-based virtual screening of phytochemicals and repurposing of FDA approved antiviral drugs unravels lead molecules as potential inhibitors of coronavirus 3C-like protease enzyme. Journal of King Saud University - Science, 2020, 32, 2845-2853.	1.6	30
22	In silico structure modelling of SARS-CoV-2 Nsp13 helicase and Nsp14 and repurposing of FDA approved antiviral drugs as dual inhibitors. Gene Reports, 2020, 21, 100860.	0.4	55
23	High-throughput virtual screening of novel potent inhibitor(s) for Human Vanin-1 enzyme. Journal of Biomolecular Structure and Dynamics, 2020, , 1-16.	2.0	1
24	In silico screening of FDA approved drugs reveals ergotamine and dihydroergotamine as potential coronavirus main protease enzyme inhibitors. Saudi Journal of Biological Sciences, 2020, 27, 2674-2682.	1.8	18
25	Analysis of the Bioactive Metabolites of the Endangered Mexican Lost Fungi Campanophyllum â€“ A Report from India. Mycobiology, 2020, 48, 58-69.	0.6	4
26	Molecular docking elucidates the plausible mechanisms underlying the anticancer properties of acetyldigitoxigenin from Adenium obesum. Saudi Journal of Biological Sciences, 2020, 27, 1907-1911.	1.8	6
27	Unravelling lead antiviral phytochemicals for the inhibition of SARS-CoV-2 Mpro enzyme through in silico approach. Life Sciences, 2020, 255, 117831.	2.0	132
28	Dissecting molecular evolutionary relationship of Krameriaceae inferred from phylotranscriptomic analysis. Bangladesh Journal of Plant Taxonomy, 2020, 27, 427-433.	0.1	3
29	Bioprospection of antiâ€inflammatory phytochemicals suggests rutaecarpine and quinine as promising 15â€lipoxygenase inhibitors. Journal of Cellular Biochemistry, 2019, 120, 13598-13613.	1.2	4
30	Discovery of novel drug candidates for inhibition of soluble epoxide hydrolase of arachidonic acid cascade pathway implicated in atherosclerosis. Computational Biology and Chemistry, 2018, 74, 1-11.	1.1	13
31	Met117 oxidation leads to enhanced flexibility of cardiovascular biomarker- lipoprotein- associated phospholipase A2 and reduced substrate binding affinity with platelet-activating factor. International Journal of Biological Macromolecules, 2018, 112, 831-840.	3.6	5
32	Impact of tyrosine nitration at positions Tyr307 and Tyr335 on structural dynamics of Lipoprotein-associated phospholipase A2â€“A therapeutically important cardiovascular biomarker for atherosclerosis. International Journal of Biological Macromolecules, 2018, 107, 1956-1964.	3.6	8
33	Correlation of cholinergic drug induced quenching of acetylcholinesterase bound thioflavin-T fluorescence with their inhibition activity. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 189, 250-257.	2.0	8
34	Impact of a nonâ€synonymous Q281R polymorphism on structure of human Lipoproteinâ€Associated Phospholipase A₂ (Lpâ€PLA₂). Journal of Cellular Biochemistry, 2018, 119, 7009-7021.	1.2	4
35	Anin silicoapproach to understand the structureâ€“function properties of a serine protease (Bacifrinase) fromBacillus cereusand experimental evidence to support the interaction of Bacifrinase with fibrinogen and thrombin. Journal of Biomolecular Structure and Dynamics, 2017, 35, 622-644.	2.0	7
36	Binding of small molecules at interface of proteinâ€“protein complex â€“ A newer approach to rational drug design. Saudi Journal of Biological Sciences, 2017, 24, 379-388.	1.8	19

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37	Disruption of redox catalytic functions of peroxiredoxin-thioredoxin complex in Mycobacterium tuberculosis H37Rv using small interface binding molecules. Computational Biology and Chemistry, 2017, 67, 69-83.	1.1	3
38	Structure based virtual screening identifies Pranlukast as a potential inhibitor against Plasmodium falciparum Adenosine Deaminase enzyme. Gene Reports, 2017, 6, 54-66.	0.4	3
39	Serum albumin interaction with xanthine drugs at nano-bio interfaces: A combined multi-spectroscopic and molecular modelling approach. Journal of Molecular Liquids, 2017, 242, 919-927.	2.3	10
40	Identification of molecular descriptors for design of novel Isoalloxazine derivatives as potential Acetylcholinesterase inhibitors against Alzheimerâ€™s disease. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1729-1742.	2.0	15
41	Exploring the physicochemical profile and the binding patterns of selected novel anticancer Himalayan plant derived active compounds with macromolecular targets. Informatics in Medicine Unlocked, 2016, 5, 1-14.	1.9	40
42	Human serum albumin reduces the potency of acetylcholinesterase inhibitor based drugs for Alzheimer's disease. Chemico-Biological Interactions, 2016, 249, 1-9.	1.7	15
43	Interactome analysis and design of inhibitors against selected protein targets of Ser/Thr protein kinase (STPK) signaling pathways in Mycobacterium tuberculosis H37Rv. Genetics and Molecular Research, 2015, 14, 10390-10403.	0.3	6