

Arun Bahadur Gurung

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/4603955/publications.pdf>

Version: 2024-02-01

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	Unravelling lead antiviral phytochemicals for the inhibition of SARS-CoV-2 Mpro enzyme through in silico approach. <i>Life Sciences</i> , 2020, 255, 117831.	2.0	132
2	An Updated Review of Computer-Aided Drug Design and Its Application to COVID-19. <i>BioMed Research International</i> , 2021, 2021, 1-18.	0.9	95
3	In silico structure modelling of SARS-CoV-2 Nsp13 helicase and Nsp14 and repurposing of FDA approved antiviral drugs as dual inhibitors. <i>Gene Reports</i> , 2020, 21, 100860.	0.4	55
4	Exploring the physicochemical profile and the binding patterns of selected novel anticancer Himalayan plant derived active compounds with macromolecular targets. <i>Informatics in Medicine Unlocked</i> , 2016, 5, 1-14.	1.9	40
5	Molecular docking and dynamics simulation study of bioactive compounds from <i>Ficus carica</i> L. with important anticancer drug targets. <i>PLoS ONE</i> , 2021, 16, e0254035.	1.1	32
6	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. <i>Journal of King Saud University - Science</i> , 2020, 32, 2845-2853.	1.6	30
7	Binding of small molecules at interface of proteinâ€“protein complex â€“ A newer approach to rational drug design. <i>Saudi Journal of Biological Sciences</i> , 2017, 24, 379-388.	1.8	19
8	In silico screening of FDA approved drugs reveals ergotamine and dihydroergotamine as potential coronavirus main protease enzyme inhibitors. <i>Saudi Journal of Biological Sciences</i> , 2020, 27, 2674-2682.	1.8	18
9	Human serum albumin reduces the potency of acetylcholinesterase inhibitor based drugs for Alzheimer's disease. <i>Chemico-Biological Interactions</i> , 2016, 249, 1-9.	1.7	15
10	Identification of molecular descriptors for design of novel Isoalloxazine derivatives as potential Acetylcholinesterase inhibitors against Alzheimerâ€™s disease. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017, 35, 1729-1742.	2.0	15
11	In silico analyses of major active constituents of fingerroot (<i>Boesenbergia rotunda</i>) unveils inhibitory activities against SARS-CoV-2 main protease enzyme. <i>Saudi Journal of Biological Sciences</i> , 2022, 29, 65-74.	1.8	14
12	Discovery of novel drug candidates for inhibition of soluble epoxide hydrolase of arachidonic acid cascade pathway implicated in atherosclerosis. <i>Computational Biology and Chemistry</i> , 2018, 74, 1-11.	1.1	13
13	Identification of SARS-CoV-2 inhibitors from extracts of <i>Houttuynia cordata</i> Thunb.. <i>Saudi Journal of Biological Sciences</i> , 2021, 28, 7517-7527.	1.8	13
14	The potential of Paritaprevir and Emetine as inhibitors of SARS-CoV-2 RdRp. <i>Saudi Journal of Biological Sciences</i> , 2021, 28, 1426-1432.	1.8	11
15	Identification of potential SARS-CoV-2 entry inhibitors by targeting the interface region between the spike RBD and human ACE2. <i>Journal of Infection and Public Health</i> , 2021, 14, 227-237.	1.9	11
16	An in silico approach unveils the potential of antiviral compounds in preclinical and clinical trials as SARS-CoV-2 omicron inhibitors. <i>Saudi Journal of Biological Sciences</i> , 2022, 29, 103297.	1.8	11
17	Serum albumin interaction with xanthine drugs at nano-bio interfaces: A combined multi-spectroscopic and molecular modelling approach. <i>Journal of Molecular Liquids</i> , 2017, 242, 919-927.	2.3	10
18	Molecular modelling studies unveil potential binding sites on human serum albumin for selected experimental and in silico COVID-19 drug candidate molecules. <i>Saudi Journal of Biological Sciences</i> , 2022, 29, 53-64.	1.8	10

#	ARTICLE	IF	CITATIONS
19	Structural and functional insights into the major mutations of SARS-CoV-2 Spike RBD and its interaction with human ACE2 receptor. <i>Journal of King Saud University - Science</i> , 2022, 34, 101773.	1.6	9
20	Impact of tyrosine nitration at positions Tyr307 and Tyr335 on structural dynamics of Lipoprotein-associated phospholipase A2—a therapeutically important cardiovascular biomarker for atherosclerosis. <i>International Journal of Biological Macromolecules</i> , 2018, 107, 1956-1964.	3.6	8
21	Correlation of cholinergic drug induced quenching of acetylcholinesterase bound thioflavin-T fluorescence with their inhibition activity. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 189, 250-257.	2.0	8
22	Artesunate induces substantial topological alterations in the SARS-CoV-2 Nsp1 protein structure. <i>Journal of King Saud University - Science</i> , 2022, 34, 101810.	1.6	8
23	An <i>in silico</i> approach to understand the structure–function properties of a serine protease (Bacifrinase) from <i>Bacillus cereus</i> and experimental evidence to support the interaction of Bacifrinase with fibrinogen and thrombin. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017, 35, 622-644.	2.0	7
24	Interactome analysis and design of inhibitors against selected protein targets of Ser/Thr protein kinase (STPK) signaling pathways in <i>Mycobacterium tuberculosis</i> H37Rv. <i>Genetics and Molecular Research</i> , 2015, 14, 10390-10403.	0.3	6
25	Molecular docking elucidates the plausible mechanisms underlying the anticancer properties of acetyldigitoxigenin from <i>Adenium obesum</i> . <i>Saudi Journal of Biological Sciences</i> , 2020, 27, 1907-1911.	1.8	6
26	Met117 oxidation leads to enhanced flexibility of cardiovascular biomarker- lipoprotein- associated phospholipase A2 and reduced substrate binding affinity with platelet-activating factor. <i>International Journal of Biological Macromolecules</i> , 2018, 112, 831-840.	3.6	5
27	Plastome of <i>Saraca asoca</i> (Detarioideae, Fabaceae): Annotation, comparison among subfamily and molecular typing. <i>Saudi Journal of Biological Sciences</i> , 2021, 28, 1487-1493.	1.8	5
28	Impact of a non-synonymous Q281R polymorphism on structure of human Lipoprotein-Associated Phospholipase A ₂ (Lp-PLA ₂). <i>Journal of Cellular Biochemistry</i> , 2018, 119, 7009-7021.	1.2	4
29	Bioprospection of anti-inflammatory phytochemicals suggests rutaecarpine and quinine as promising 15-lipoxygenase inhibitors. <i>Journal of Cellular Biochemistry</i> , 2019, 120, 13598-13613.	1.2	4
30	Analysis of the Bioactive Metabolites of the Endangered Mexican Lost Fungi <i>Campanophyllum</i> – A Report from India. <i>Mycobiology</i> , 2020, 48, 58-69.	0.6	4
31	The cp genome characterization of <i>Adenium obesum</i> : Gene content, repeat organization and phylogeny. <i>Saudi Journal of Biological Sciences</i> , 2021, 28, 3768-3775.	1.8	4
32	RNA-Seq analysis reveals the role of MYB12, MYB111 and MBW complex repressors in regulation of flavonoid biosynthesis in stigmas of saffron (<i>Crocus sativus</i> L.) flowers. <i>Acta Physiologiae Plantarum</i> , 2022, 44, 1.	1.0	4
33	Disruption of redox catalytic functions of peroxiredoxin-thioredoxin complex in <i>Mycobacterium tuberculosis</i> H37Rv using small interface binding molecules. <i>Computational Biology and Chemistry</i> , 2017, 67, 69-83.	1.1	3
34	Structure based virtual screening identifies Pranlukast as a potential inhibitor against <i>Plasmodium falciparum</i> Adenosine Deaminase enzyme. <i>Gene Reports</i> , 2017, 6, 54-66.	0.4	3
35	<i>In silico</i> molecular modelling, structural dynamics simulation and characterization of antifungal nature of I ² -glucosidase enzyme from <i>Sechium edule</i> . <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 39, 1-9.	2.0	3
36	Dissecting molecular evolutionary relationship of Krameriaceae inferred from phylotranscriptomic analysis. <i>Bangladesh Journal of Plant Taxonomy</i> , 2020, 27, 427-433.	0.1	3

#	ARTICLE	IF	CITATIONS
37	Potential of antiviral peptide-based SARS-CoV-2 inactivators to combat COVID-19. <i>PLoS ONE</i> , 2022, 17, e0268919.	1.1	2
38	Data-mining technique identifies potential target proteins playing a dual role in inflammation and oxidative stress pathways in relation to atherosclerosis plaque development. <i>Informatics in Medicine Unlocked</i> , 2020, 18, 100278.	1.9	1
39	Identification of potential drug-like molecules for inhibition of the inflammatory activity of cyclooxygenase-2. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 5293-5306.	2.0	1
40	High-throughput virtual screening of novel potent inhibitor(s) for Human Vanin-1 enzyme. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, , 1-16.	2.0	1
41	Identification of novel drug candidates for the inhibition of catalytic cleavage activity of coronavirus 3CL-like protease enzyme. <i>Current Pharmaceutical Biotechnology</i> , 2021, 22, .	0.9	1
42	Transcriptome characterization of <i>Larrea tridentata</i> and identification of genes associated with phenylpropanoid metabolic pathways. <i>PLoS ONE</i> , 2022, 17, e0265231.	1.1	1
43	Insights into plastome of <i>Fagonia indica</i> Burm.f. (Zygophyllaceae): organization, annotation and phylogeny. <i>Saudi Journal of Biological Sciences</i> , 2022, 29, 1313-1321.	1.8	0