## Md Imtaiyaz Hassan

List of Publications by Year in descending order

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383 papers 11,458 citations

51 h-index 76898 74 g-index

390 all docs

390 docs citations

times ranked

390

9193 citing authors

#	Article	IF	CITATIONS
1	Deciphering the potent application of nanobentonite and α-Fe2O3/bentonite nanocomposite in dye removal: revisiting the insights of adsorption mechanism. Applied Nanoscience (Switzerland), 2023, 13, 883-897.	3.1	4
2	Design and development of 5-(4H)-oxazolones as potential inhibitors of human carbonic anhydrase VA: towards therapeutic management of diabetes and obesity. Journal of Biomolecular Structure and Dynamics, 2022, 40, 3144-3154.	3.5	10
3	Structure-based identification of potential SARS-CoV-2 main protease inhibitors. Journal of Biomolecular Structure and Dynamics, 2022, 40, 3595-3608.	3.5	50
4	Insight into the binding of PEG-400 with eye protein alpha-crystallin: Multi spectroscopic and computational approach: possible therapeutics targeting eye diseases. Journal of Biomolecular Structure and Dynamics, 2022, 40, 4496-4506.	3.5	19
5	Investigation of sphingosine kinase 1 inhibitory potential of cinchonine and colcemid targeting anticancer therapy. Journal of Biomolecular Structure and Dynamics, 2022, 40, 6350-6362.	3.5	10
6	Impact of non-synonymous mutations on the structure and function of telomeric repeat binding factor 1. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9053-9066.	3.5	16
7	Identification of plant-based hexokinase 2 inhibitors: combined molecular docking and dynamics simulation studies. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10319-10331.	3.5	23
8	Thymoquinone and quercetin induce enhanced apoptosis in nonâ€small cell lung cancer in combination through the Bax/Bcl2 cascade. Journal of Cellular Biochemistry, 2022, 123, 259-274.	2.6	20
9	Clinical features and mechanistic insights into drug repurposing for combating COVID-19. International Journal of Biochemistry and Cell Biology, 2022, 142, 106114.	2.8	12
10	PEG mediated destabilization of holo $\hat{l}$ ±-lactalbumin probed by <i>in silico</i> and <i>in vitro</i> studies: deviation from excluded volume effect. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13265-13277.	3.5	2
11	Myricetin inhibits breast and lung cancer cells proliferation via inhibiting MARK4. Journal of Cellular Biochemistry, 2022, 123, 359-374.	2.6	26
12	Effect of pH on the structure and stability of irisin, a multifunctional protein: Multispectroscopic and molecular dynamics simulation approach. Journal of Molecular Structure, 2022, 1252, 132141.	3.6	11
13	Containment strategies for COVID-19 in India: lessons from the second wave. Expert Review of Anti-Infective Therapy, 2022, , 1-7.	4.4	8
14	Modulatory Role of Quercetin in Mitochondrial Dysfunction in Titanium Dioxide Nanoparticle-Induced Hepatotoxicity. ACS Omega, 2022, 7, 3192-3202.	3.5	14
15	Carbonic anhydrase IX: A tumor acidification switch in heterogeneity and chemokine regulation. Seminars in Cancer Biology, 2022, 86, 899-913.	9.6	30
16	Natural products can be used in therapeutic management of COVID-19: Probable mechanistic insights. Biomedicine and Pharmacotherapy, 2022, 147, 112658.	5.6	50
17	Implications of tempol in pyruvate dehydrogenase kinase 3 targeted anticancer therapeutics: Computational, spectroscopic, and calorimetric studies. Journal of Molecular Liquids, 2022, 350, 118581.	4.9	18
18	Impact of Single Amino Acid Substitutions in Parkinsonism-Associated Deglycase-PARK7 and Their Association with Parkinson's Disease. Journal of Personalized Medicine, 2022, 12, 220.	2.5	4

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19	Differential gene expression and network analysis in head and neck squamous cell carcinoma. Molecular and Cellular Biochemistry, 2022, 477, 1361-1370.	3.1	3
20	Effect of pH on the structure and function of cyclin-dependent kinase 6. PLoS ONE, 2022, 17, e0263693.	2.5	8
21	FNDC5/Irisin: Physiology and Pathophysiology. Molecules, 2022, 27, 1118.	3.8	56
22	Bioactive phytoconstituents as potent inhibitors of casein kinase-2: dual implications in cancer and COVID-19 therapeutics. RSC Advances, 2022, 12, 7872-7882.	3.6	14
23	Therapeutic Outcomes of Isatin and Its Derivatives against Multiple Diseases: Recent Developments in Drug Discovery. Pharmaceuticals, 2022, 15, 272.	3.8	43
24	Identification of intrinsically disorder regions in non-structural proteins of SARS-CoV-2: New insights into drug and vaccine resistance. Molecular and Cellular Biochemistry, 2022, 477, 1607-1619.	3.1	11
25	Insights into the Antibacterial Activity of Prolactin-Inducible Protein against the Standard and Environmental MDR Bacterial Strains. Microorganisms, 2022, 10, 597.	3.6	3
26	Cadmium-Tolerant Plant Growth-Promoting Bacteria Curtobacterium oceanosedimentum Improves Growth Attributes and Strengthens Antioxidant System in Chili (Capsicum frutescens). Sustainability, 2022, 14, 4335.	3.2	12
27	Target-Based Virtual Screening of Natural Compounds Identifies a Potent Antimalarial With Selective Falcipain-2 Inhibitory Activity. Frontiers in Pharmacology, 2022, 13, 850176.	3.5	4
28	Biomedical features and therapeutic potential of rosmarinic acid. Archives of Pharmacal Research, 2022, 45, 205-228.	6.3	51
29	Inhibition of PDK3 by artemisinin, a repurposed antimalarial drug in cancer therapy. Journal of Molecular Liquids, 2022, 355, 118928.	4.9	16
30	Exploring binding mechanism of naringenin to human transferrin using combined spectroscopic and computational methods: Towards therapeutic targeting of neurodegenerative diseases. Journal of Molecular Liquids, 2022, 356, 119001.	4.9	9
31	Inhibition of MARK4 by serotonin as an attractive therapeutic approach to combat Alzheimer's disease and neuroinflammation. RSC Medicinal Chemistry, 2022, 13, 737-745.	3.9	12
32	Comparative analysis of web-based programs for single amino acid substitutions in proteins. PLoS ONE, 2022, 17, e0267084.	2.5	6
33	Bioactive Phytoconstituents as Potent Inhibitors of Tyrosine-Protein Kinase Yes (YES1): Implications in Anticancer Therapeutics. Molecules, 2022, 27, 3060.	3.8	10
34	Infection Dynamics of ATG8 in Leishmania: Balancing Autophagy for Therapeutics. Molecules, 2022, 27, 3142.	3.8	6
35	Unraveling the Binding Mechanism of Alzheimer's Drugs with Irisin: Spectroscopic, Calorimetric, and Computational Approaches. International Journal of Molecular Sciences, 2022, 23, 5965.	4.1	7
36	Investigating binding mechanism of thymoquinone to human transferrin, targeting Alzheimer's disease therapy. Journal of Cellular Biochemistry, 2022, 123, 1381-1393.	2.6	12

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37	Discovering Tuberosin and Villosol as Potent and Selective Inhibitors of AKT1 for Therapeutic Targeting of Oral Squamous Cell Carcinoma. Journal of Personalized Medicine, 2022, 12, 1083.	2.5	3
38	Inhibiting Cyclin-Dependent Kinase 6 by Taurine: Implications in Anticancer Therapeutics. ACS Omega, 2022, 7, 25844-25852.	<b>3.</b> 5	10
39	Frustration analysis of TBK1 missense mutations reported in ALS/FTD and cancer patients. 3 Biotech, 2022, 12, .	2.2	4
40	Death-Associated Protein Kinase 3 Inhibitors Identified by Virtual Screening for Drug Discovery in Cancer and Hypertension. OMICS A Journal of Integrative Biology, 2022, 26, 404-413.	2.0	7
41	Insight into the Conformational Transitions of Serine Acetyl Transferase Isoforms in <i>E. histolytica</i> : Implications for Structural and Functional Balance. ACS Omega, 2022, 7, 24626-24637.	3 <b>.</b> 5	0
42	Unravelling the unfolding pathway of human Fas-activated serine/threonine kinase induced by urea. Journal of Biomolecular Structure and Dynamics, 2021, 39, 5516-5525.	3 <b>.</b> 5	1
43	InstaDock: A single-click graphical user interface for molecular docking-based virtual high-throughput screening. Briefings in Bioinformatics, 2021, 22, .	<b>6.</b> 5	127
44	Impact of glioblastoma multiforme associated mutations on the structure and function of MAP/microtubule affinity regulating kinase 4. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1781-1794.	3 <b>.</b> 5	8
45	SARS-CoV-2 mediated lung inflammatory responses in host: targeting the cytokine storm for therapeutic interventions. Molecular and Cellular Biochemistry, 2021, 476, 675-687.	3.1	38
46	Capping agent-induced variation of physicochemical and biological properties of α-Fe2O3 nanoparticles. Materials Chemistry and Physics, 2021, 258, 123899.	4.0	26
47	Emerging role of protein kinases in diabetes mellitus: From mechanism to therapy. Advances in Protein Chemistry and Structural Biology, 2021, 124, 47-85.	2.3	4
48	Polo-like Kinase $1$ as an emerging drug target: structure, function and therapeutic implications. Journal of Drug Targeting, 2021, 29, 168-184.	4.4	30
49	Diagnostic approaches in COVID-19: clinical updates. Expert Review of Respiratory Medicine, 2021, 15, 197-212.	2.5	43
50	Targeting metacaspase-3 from <i>Plasmodium falciparum</i> towards antimalarial therapy: A combined approach of <i>in-silico</i> and <i>in-vitro</i> investigation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 421-430.	<b>3.</b> 5	6
51	Investigation of conformational dynamics of Tyr89Cys mutation in protection of telomeres 1 gene associated with familial melanoma. Journal of Biomolecular Structure and Dynamics, 2021, 39, 35-44.	<b>3.</b> 5	18
52	Identification of high-affinity inhibitors of pyruvate dehydrogenase kinase-3: towards therapeutic management of cancer. Journal of Biomolecular Structure and Dynamics, 2021, 39, 586-594.	3.5	22
53	Heparin Accelerates the Protein Aggregation via the Downhill Polymerization Mechanism: Multi-Spectroscopic Studies to Delineate the Implications on Proteinopathies. ACS Omega, 2021, 6, 2328-2339.	3 <b>.</b> 5	20
54	Emerging therapeutic approaches to COVID-19. Current Pharmaceutical Design, 2021, 27, 3370-3388.	1.9	2

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55	Guidelines and Safety Considerations in the Laboratory Diagnosis of SARS-CoV-2 Infection: A Prerequisite Study for Health Professionals. Risk Management and Healthcare Policy, 2021, Volume 14, 379-389.	2.5	19
56	Trehalose Restrains the Fibril Load towards $\hat{l}$ ±-Lactalbumin Aggregation and Halts Fibrillation in a Concentration-Dependent Manner. Biomolecules, 2021, 11, 414.	4.0	11
57	Mechanistic insights into the pathogenesis of neurodegenerative diseases: towards the development of effective therapy. Molecular and Cellular Biochemistry, 2021, 476, 2739-2752.	3.1	12
58	Multispectroscopic and Molecular Docking Insight into Elucidating the Interaction of Irisin with Rivastigmine Tartrate: A Combinational Therapy Approach to Fight Alzheimer's Disease. ACS Omega, 2021, 6, 7910-7921.	3.5	13
59	A computational study on active constituents of Habb-ul-aas and Tabasheer as inhibitors of SARS-CoV-2 main protease. Journal of Biomolecular Structure and Dynamics, 2021, , 1-12.	3.5	5
60	Elucidating the Interaction of Human Ferritin with Quercetin and Naringenin: Implication of Natural Products in Neurodegenerative Diseases: Molecular Docking and Dynamics Simulation Insight. ACS Omega, 2021, 6, 7922-7930.	3.5	45
61	Interaction of polyethylene glycol with cytochrome c investigated via in vitro and in silico approaches. Scientific Reports, 2021, 11, 6475.	3.3	26
62	Design and development of novel inhibitors of aldo-ketoreductase 1C1 as potential lead molecules in treatment of breast cancer. Molecular and Cellular Biochemistry, 2021, 476, 2975-2987.	3.1	5
63	Stability of uniformly labeled (13C and 15N) cytochrome c and its L94G mutant. Scientific Reports, 2021, 11, 6804.	3.3	3
64	Structural insights into the transient closed conformation and pH dependent ATPase activity of S.Typhi GyraseB N- terminal domain. Archives of Biochemistry and Biophysics, 2021, 701, 108786.	3.0	3
65	Identification of natural compounds as potent inhibitors of SARS-CoV-2 main protease using combined docking and molecular dynamics simulations. Saudi Journal of Biological Sciences, 2021, 28, 2423-2431.	3.8	47
66	Potential drug targets of SARS-CoV-2: From genomics to therapeutics. International Journal of Biological Macromolecules, 2021, 177, 1-9.	7.5	77
67	Targeting the Sphingosine Kinase/Sphingosine-1-Phosphate Signaling Axis in Drug Discovery for Cancer Therapy. Cancers, 2021, 13, 1898.	3.7	33
68	Targeting cyclinâ€dependent kinase 6 by vanillin inhibits proliferation of breast and lung cancer cells: Combined computational and biochemical studies. Journal of Cellular Biochemistry, 2021, 122, 897-910.	2.6	25
69	Structural Refolding and Thermal Stability of Myoglobin in the Presence of Mixture of Crowders: Importance of Various Interactions for Protein Stabilization in Crowded Conditions. Molecules, 2021, 26, 2807.	3.8	12
70	Structural genomics approach to investigate deleterious impact of nsSNPs in conserved telomere maintenance component 1. Scientific Reports, 2021, 11, 10202.	3.3	18
71	Aurora B kinase: a potential drug target for cancer therapy. Journal of Cancer Research and Clinical Oncology, 2021, 147, 2187-2198.	2.5	12
72	5-Fluorouracil (5-FU)-based Aza-Michael addition product: A selective carbonic anhydrase IX inhibitor. Journal of Molecular Structure, 2021, 1231, 129977.	3.6	7

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73	Crowding Milleu stabilizes apo-myoglobin against chemical-induced denaturation: Dominance of hardcore repulsions in the heme devoid protein. International Journal of Biological Macromolecules, 2021, 181, 552-560.	7.5	6
74	Structureâ€based investigation of MARK4 inhibitory potential of Naringenin for therapeutic management of cancer and neurodegenerative diseases. Journal of Cellular Biochemistry, 2021, 122, 1445-1459.	2.6	44
75	Design, synthesis, and biological evaluation of novel benzimidazole derivatives as sphingosine kinase 1 inhibitor. Archiv Der Pharmazie, 2021, 354, e2100080.	4.1	6
76	Design and synthesis of new pyrazolylbenzimidazoles as sphingosine kinase-1 inhibitors. Medicinal Chemistry Research, 2021, 30, 1614-1634.	2.4	3
77	Mechanistic insight into the binding of graphene oxide with human serum albumin: Multispectroscopic and molecular docking approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 256, 119750.	3.9	21
78	A review on the role of TANK-binding kinase 1 signaling in cancer. International Journal of Biological Macromolecules, 2021, 183, 2364-2375.	<b>7.</b> 5	28
79	Impact of single amino acid substitution on the structure and function of TANKâ€binding kinaseâ€1. Journal of Cellular Biochemistry, 2021, 122, 1475-1490.	2.6	11
80	Sequence and structure-based method to predict diacylglycerol lipases in protein sequence. International Journal of Biological Macromolecules, 2021, 182, 455-463.	<b>7.</b> 5	2
81	Vitamin D and lumisterol novel metabolites can inhibit SARS-CoV-2 replication machinery enzymes. American Journal of Physiology - Endocrinology and Metabolism, 2021, 321, E246-E251.	3.5	38
82	Plant cytochrome P450s: Role in stress tolerance and potential applications for human welfare. International Journal of Biological Macromolecules, 2021, 184, 874-886.	7.5	16
83	Discovery of Natural Compounds as Potential Inhibitors of Human Carbonic Anhydrase II: An Integrated Virtual Screening, Docking, and Molecular Dynamics Simulation Study. OMICS A Journal of Integrative Biology, 2021, 25, 513-524.	2.0	12
84	Targeting pyruvate dehydrogenase kinase signaling in the development of effective cancer therapy. Biochimica Et Biophysica Acta: Reviews on Cancer, 2021, 1876, 188568.	7.4	75
85	Exploring the molecular interactions of Galantamine with human Transferrin: In-silico and in vitro insight. Journal of Molecular Liquids, 2021, 335, 116227.	4.9	8
86	B Cell Lymphoma 2: A Potential Therapeutic Target for Cancer Therapy. International Journal of Molecular Sciences, 2021, 22, 10442.	4.1	39
87	Phytoconstituents and Medicinal Plants for Anticancer Drug Discovery: Computational Identification of Potent Inhibitors of PIM1 Kinase. OMICS A Journal of Integrative Biology, 2021, 25, 580-590.	2.0	30
88	Implications of the second wave of COVID-19 in India. Lancet Respiratory Medicine, the, 2021, 9, e93-e94.	10.7	106
89	Macrophage Activation Syndrome and COVID 19: Impact of MAPK Driven Immune-Epigenetic Programming by SARS-Cov-2. Frontiers in Immunology, 2021, 12, 763313.	4.8	18
90	Probing the interaction of memantine, an important Alzheimer's drug, with human serum albumin: In silico and in vitro approach. Journal of Molecular Liquids, 2021, 340, 116888.	4.9	26

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91	Therapeutic targeting of PIM KINASE signaling in cancer therapy: Structural and clinical prospects. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129995.	2.4	16
92	Characterization of different intermediate states in myoglobin induced by polyethylene glycol: A process of spontaneous molecular self-organization foresees the energy landscape theory via in vitro and in silico approaches. Journal of Molecular Liquids, 2021, 342, 117502.	4.9	9
93	Spectroscopic, calorimetric and in silico insight into the molecular interactions of Memantine with human transferrin: Implications of Alzheimer's drugs. International Journal of Biological Macromolecules, 2021, 190, 660-666.	<b>7.</b> 5	8
94	MAP/Microtubule Affinity Regulating Kinase 4 Inhibitory Potential of Irisin: A New Therapeutic Strategy to Combat Cancer and Alzheimer's Disease. International Journal of Molecular Sciences, 2021, 22, 10986.	4.1	25
95	Genomic Variations in the Structural Proteins of SARS-CoV-2 and Their Deleterious Impact on Pathogenesis: A Comparative Genomics Approach. Frontiers in Cellular and Infection Microbiology, 2021, 11, 765039.	3.9	43
96	Mechanistic insights into the role of serum-glucocorticoid kinase 1 in diabetic nephropathy: A systematic review. International Journal of Biological Macromolecules, 2021, 193, 562-573.	7.5	5
97	Ultra-sensitive techniques for detecting neurological biomarkers: Prospects for early diagnosis. Biochemical and Biophysical Research Communications, 2021, 584, 15-18.	2.1	4
98	Investigating single amino acid substitutions in PIM1 kinase: A structural genomics approach. PLoS ONE, 2021, 16, e0258929.	2.5	13
99	Impact of Deleterious Mutations on Structure, Function and Stability of Serum/Glucocorticoid Regulated Kinase 1: A Gene to Diseases Correlation. Frontiers in Molecular Biosciences, 2021, 8, 780284.	3 <b>.</b> 5	12
100	Therapeutic Potential of Ursolic Acid in Cancer and Diabetic Neuropathy Diseases. International Journal of Molecular Sciences, 2021, 22, 12162.	4.1	42
101	Functional and Structural Characterization of Pediococcus pentosaceus-Derived Biosurfactant and Its Biomedical Potential against Bacterial Adhesion, Quorum Sensing, and Biofilm Formation. Antibiotics, 2021, 10, 1371.	3.7	21
102	Delineating the Aggregation-Prone Hotspot Regions (Peptides) in the Human Cu/Zn Superoxide Dismutase 1. ACS Omega, 2021, 6, 33985-33994.	3.5	1
103	Neurodegenerative brain models vs. cell replacement or restoration therapy: A review on promises and pitfalls. Biochemical and Biophysical Research Communications, 2021, 585, 124-131.	2.1	5
104	Investigating host-virus interaction mechanism and phylogenetic analysis of viral proteins involved in the pathogenesis. PLoS ONE, 2021, 16, e0261497.	2.5	2
105	$\hat{l}^2$ 2-spectrin (SPTBN1) as a therapeutic target for diet-induced liver disease and preventing cancer development. Science Translational Medicine, 2021, 13, eabk2267.	12.4	23
106	Identification of Phytoconstituents as Potent Inhibitors of Casein Kinase-1 Alpha Using Virtual Screening and Molecular Dynamics Simulations. Pharmaceutics, 2021, 13, 2157.	4.5	25
107	Impact of Gln94Glu mutation on the structure and function of protection of telomere 1, a cause of cutaneous familial melanoma. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1514-1524.	3.5	29
108	Spectroscopic, calorimetric and molecular docking insight into the interaction of Alzheimer's drug donepezil with human transferrin: implications of Alzheimer's drug. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1094-1102.	3 <b>.</b> 5	60

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109	Mutated CEACAMs Disrupt Transforming Growth Factor Beta Signaling and Alter the Intestinal Microbiome to Promote Colorectal Carcinogenesis. Gastroenterology, 2020, 158, 238-252.	1.3	46
110	Functional implications of pH-induced conformational changes in the Sphingosine kinase 1. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 225, 117453.	3.9	44
111	Virtual high-throughput screening of natural compounds in-search of potential inhibitors for protection of telomeres 1 (POT1). Journal of Biomolecular Structure and Dynamics, 2020, 38, 4625-4634.	3.5	32
112	The structural basis of acid resistance in <i>Mycobacterium tuberculosis</i> pH regime molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4483-4492.	3.5	3
113	Identification and evaluation of glutathione conjugate gamma- <scp>Identification and evaluation of glutathione conjugate gamma-<scp>Identification and Dynamics, 2020, 38, 3610-3620.</scp></scp>	3.5	46
114	Evaluation of pyrazolopyrimidine derivatives as microtubule affinity regulating kinase 4 inhibitors: Towards therapeutic management of Alzheimer's disease. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3892-3907.	3.5	37
115	Backbone and side chain 1H, 15N and 13C chemical shift assignments of the molten globule state of L94G mutant of horse cytochrome-c. Biomolecular NMR Assignments, 2020, 14, 37-44.	0.8	1
116	Investigation of guanidinium chloride-induced unfolding pathway of sphingosine kinase 1. International Journal of Biological Macromolecules, 2020, 147, 177-186.	7.5	12
117	Pharmacological Activities of Novel Chromene Derivatives as Calcium/Calmodulin Dependent Protein Kinase IV (CAMKIV) Inhibitors. ChemistrySelect, 2020, 5, 498-505.	1.5	4
118	Amphiphilic nature of polyethylene glycols and their role in medical research. Polymer Testing, 2020, 82, 106316.	4.8	45
119	Urea Stress: Myo-inositol's efficacy to counteract destabilization of TIM- $\hat{I}^2$ -globin complex by urea is as good as that of the methylamine. International Journal of Biological Macromolecules, 2020, 151, 1108-1115.	7.5	3
120	Molecular and macromolecular crowding-induced stabilization of proteins: Effect of dextran and its building block alone and their mixtures on stability and structure of lysozyme. International Journal of Biological Macromolecules, 2020, 150, 1238-1248.	7.5	18
121	Functional and Structural Analysis of Predicted Proteins Obtained from Homo sapiens' Minisatellite 33.15-Tagged Transcript pAKT-45 Variants. BioMed Research International, 2020, 2020, 1-9.	1.9	1
122	Inhibiting CDK6 Activity by Quercetin Is an Attractive Strategy for Cancer Therapy. ACS Omega, 2020, 5, 27480-27491.	3.5	48
123	Chitin and its derivatives: Structural properties and biomedical applications. International Journal of Biological Macromolecules, 2020, 164, 526-539.	7.5	105
124	Evaluation of Binding of Rosmarinic Acid with Human Transferrin and Its Impact on the Protein Structure: Targeting Polyphenolic Acid-Induced Protection of Neurodegenerative Disorders. Oxidative Medicine and Cellular Longevity, 2020, 2020, 1-14.	4.0	26
125	Heme-iron ligand (M80-Fe) in cytochrome c is destabilizing: combined in $\hat{A}$ vitro and in silico approaches to monitor changes in structure, stability and dynamics of the protein on mutation. Journal of Biomolecular Structure and Dynamics, 2020, , $1$ -18.	3.5	11
126	Mechanistic insights into the urea-induced denaturation of human sphingosine kinase 1. International Journal of Biological Macromolecules, 2020, 161, 1496-1505.	7.5	14

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127	Impact of amino acid substitution in the kinase domain of Bruton tyrosine kinase and its association with X-linked agammaglobulinemia. International Journal of Biological Macromolecules, 2020, 164, 2399-2408.	7.5	18
128	Conformational changes in cytochrome c directed by ethylene glycol accompanying complex formation: Protein-solvent preferential interaction or/and kosmotropic effect. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 242, 118788.	3.9	11
129	Identification and structure–activity relationship (SAR) studies of carvacrol derivatives as potential anti-malarial against Plasmodium falciparum falcipain-2 protease. Bioorganic Chemistry, 2020, 103, 104142.	4.1	16
130	Concentration dependent effect of ethylene glycol on the structure and stability of holo $\hat{l}_{\pm}$ -lactalbumin: Characterization of intermediate state amidst soft interactions. International Journal of Biological Macromolecules, 2020, 164, 2151-2161.	7.5	6
131	Identification of high-affinity inhibitors of SARS-CoV-2 main protease: Towards the development of effective COVID-19 therapy. Virus Research, 2020, 288, 198102.	2.2	79
132	A Systems View of the Genome Guardians: Mapping the Signaling Circuitry Underlying Oligonucleotide/Oligosaccharide-Binding Fold Proteins. OMICS A Journal of Integrative Biology, 2020, 24, 518-530.	2.0	2
133	Impact of Hydroxychloroquine/Chloroquine in COVID-19 Therapy: Two Sides of the Coin. Journal of Interferon and Cytokine Research, 2020, 40, 469-471.	1.2	18
134	Identification of Potential Inhibitors of Calcium/Calmodulin-Dependent Protein Kinase IV from Bioactive Phytoconstituents. Oxidative Medicine and Cellular Longevity, 2020, 2020, 1-14.	4.0	39
135	Identification of morpholine based hydroxylamine analogues: selective inhibitors of MARK4/Par-1d causing cancer cell death through apoptosis. New Journal of Chemistry, 2020, 44, 16626-16637.	2.8	13
136	Molecular Basis of Pathogenesis of Coronaviruses: A Comparative Genomics Approach to Planetary Health to Prevent Zoonotic Outbreaks in the 21st Century. OMICS A Journal of Integrative Biology, 2020, 24, 634-644.	2.0	41
137	Design and Development of Small-Molecule Arylaldoxime/5-Nitroimidazole Hybrids as Potent Inhibitors of MARK4: A Promising Approach for Target-Based Cancer Therapy. ACS Omega, 2020, 5, 22759-22771.	3.5	16
138	Biophysical Insights into Implications of PEG-400 on the $\hat{l}\pm$ -Crystallin Structure: Multispectroscopic and Microscopic Approach. ACS Omega, 2020, 5, 19210-19216.	3.5	7
139	Discovery of Harmaline as a Potent Inhibitor of Sphingosine Kinase-1: A Chemopreventive Role in Lung Cancer. ACS Omega, 2020, 5, 21550-21560.	3.5	35
140	Structural analyses and classification of novel isoniazid resistance coupled mutational landscapes in Mycobacterium tuberculosis: a combined molecular docking and MD simulation study. Journal of Biomolecular Structure and Dynamics, 2020, , 1-10.	3.5	2
141	Biophysical Elucidation of Fibrillation Inhibition by Sugar Osmolytes in α-Lactalbumin: Multispectroscopic and Molecular Docking Approaches. ACS Omega, 2020, 5, 26871-26882.	3.5	23
142	Ellagic Acid Controls Cell Proliferation and Induces Apoptosis in Breast Cancer Cells via Inhibition of Cyclin-Dependent Kinase 6. International Journal of Molecular Sciences, 2020, 21, 3526.	4.1	74
143	Structure, function and therapeutic implications of OB-fold proteins: A lesson from past to present. Briefings in Functional Genomics, 2020, 19, 377-389.	2.7	6
144	Classification and functional analyses of putative virulence factors of Mycobacterium tuberculosis: A combined sequence and structure based study. Computational Biology and Chemistry, 2020, 87, 107270.	2.3	0

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145	Discovery of Hordenine as a Potential Inhibitor of Pyruvate Dehydrogenase Kinase 3: Implication in Lung Cancer Therapy. Biomedicines, 2020, 8, 119.	3.2	76
146	Mechanistic insights into the urea-induced denaturation of a non-seleno thiol specific antioxidant human peroxiredoxin 6. International Journal of Biological Macromolecules, 2020, 161, 1171-1180.	<b>7.</b> 5	9
147	Molecular Modeling of Chemosensory Protein 3 from Spodoptera litura and Its Binding Property with Plant Defensive Metabolites. International Journal of Molecular Sciences, 2020, 21, 4073.	4.1	13
148	Identification of Sphingosine Kinase-1 Inhibitors from Bioactive Natural Products Targeting Cancer Therapy. ACS Omega, 2020, 5, 14720-14729.	3.5	38
149	Insights into the Conserved Regulatory Mechanisms of Human and Yeast Aging. Biomolecules, 2020, 10, 882.	4.0	15
150	Effects of Ethylene Glycol on the Structure and Stability of Myoglobin Using Spectroscopic, Interaction, and <i>In Silico</i> Approaches: Monomer Is Different from Those of Its Polymers. ACS Omega, 2020, 5, 13840-13850.	3.5	21
151	Design and Development of Novel Urea, Sulfonyltriurea, and Sulfonamide Derivatives as Potential Inhibitors of Sphingosine Kinase 1. Pharmaceuticals, 2020, 13, 118.	3.8	13
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