Taj Mohammad

List of Publications by Year
in descending order

81 papers	3,501 citations	147566 31 h-index	161609 54 g-index
82 all docs	82 docs citations	82 times ranked	3029 citing authors

#	Article	IF	Citations
1	Insights into SARS-CoV-2 genome, structure, evolution, pathogenesis and therapies: Structural genomics approach. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2020, 1866, 165878.	1.8	770
2	Advancements in Docking and Molecular Dynamics Simulations Towards Ligand-receptor Interactions and Structure-function Relationships. Current Topics in Medicinal Chemistry, 2018, 18, 1755-1768.	1.0	188
3	Glecaprevir and Maraviroc are high-affinity inhibitors of SARS-CoV-2 main protease: possible implication in COVID-19 therapy. Bioscience Reports, 2020, 40, .	1.1	129
4	InstaDock: A single-click graphical user interface for molecular docking-based virtual high-throughput screening. Briefings in Bioinformatics, 2021, 22, .	3.2	127
5	Identification and evaluation of bioactive natural products as potential inhibitors of human microtubule affinity-regulating kinase 4 (MARK4). Journal of Biomolecular Structure and Dynamics, 2019, 37, 1813-1829.	2.0	114
6	Investigation of molecular mechanism of recognition between citral and MARK4: A newer therapeutic approach to attenuate cancer cell progression. International Journal of Biological Macromolecules, 2018, 107, 2580-2589.	3.6	96
7	Virtual Screening Approach to Identify High-Affinity Inhibitors of Serum and Glucocorticoid-Regulated Kinase 1 among Bioactive Natural Products: Combined Molecular Docking and Simulation Studies. Molecules, 2020, 25, 823.	1.7	89
8	Investigation of inhibitory potential of quercetin to the pyruvate dehydrogenase kinase 3: Towards implications in anticancer therapy. International Journal of Biological Macromolecules, 2019, 136, 1076-1085.	3.6	80
9	Identification of high-affinity inhibitors of SARS-CoV-2 main protease: Towards the development of effective COVID-19 therapy. Virus Research, 2020, 288, 198102.	1.1	79
10	Evaluation of ellagic acid as an inhibitor of sphingosine kinase 1: A targeted approach towards anticancer therapy. Biomedicine and Pharmacotherapy, 2019, 118, 109245.	2.5	78
11	Potential drug targets of SARS-CoV-2: From genomics to therapeutics. International Journal of Biological Macromolecules, 2021, 177, 1-9.	3.6	77
12	Discovery of Hordenine as a Potential Inhibitor of Pyruvate Dehydrogenase Kinase 3: Implication in Lung Cancer Therapy. Biomedicines, 2020, 8, 119.	1.4	76
13	MARK4 Inhibited by AChE Inhibitors, Donepezil and Rivastigmine Tartrate: Insights into Alzheimerâ€™s Disease Therapy. Biomolecules, 2020, 10, 789.	1.8	76
14	Targeting pyruvate dehydrogenase kinase signaling in the development of effective cancer therapy. Biochimica Et Biophysica Acta: Reviews on Cancer, 2021, 1876, 188568.	3.3	75
15	Identification and Evaluation of Inhibitors of Lipase from Malassezia restricta using Virtual High-Throughput Screening and Molecular Dynamics Studies. International Journal of Molecular Sciences, 2019, 20, 884.	1.8	72
16	Identification of Î±-Mangostin as a Potential Inhibitor of Microtubule Affinity Regulating Kinase 4. Journal of Natural Products, 2019, 82, 2252-2261.	1.5	62
17	FNDC5/Irisin: Physiology and Pathophysiology. Molecules, 2022, 27, 1118.	1.7	56
18	Structural Analysis and Conformational Dynamics of STN1 Gene Mutations Involved in Coat Plus Syndrome. Frontiers in Molecular Biosciences, 2019, 6, 41.	1.6	53

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19	Evaluation of binding and inhibition mechanism of dietary phytochemicals with sphingosine kinase 1: Towards targeted anticancer therapy. Scientific Reports, 2019, 9, 18727.	1.6	52
20	Probing the interaction of Rivastigmine Tartrate, an important Alzheimer's drug, with serum albumin: Attempting treatment of Alzheimer's disease. International Journal of Biological Macromolecules, 2020, 148, 533-542.	3.6	52
21	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.	1.8	47
22	Unraveling Binding Mechanism of Alzheimerâ€™s Drug Rivastigmine Tartrate with Human Transferrin: Molecular Docking and Multi-Spectroscopic Approach towards Neurodegenerative Diseases. Biomolecules, 2019, 9, 495.	1.8	46
23	Mutated CEACAMs Disrupt Transforming Growth Factor Beta Signaling and Alter the Intestinal Microbiome to Promote Colorectal Carcinogenesis. Gastroenterology, 2020, 158, 238-252.	0.6	46
24	Identification and evaluation of glutathione conjugate gamma-<scp>l</scp>-glutamyl-<scp>l</scp>-cysteine for improved drug delivery to the brain. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3610-3620.	2.0	46
25	Exploring molecular insights into the interaction mechanism of cholesterol derivatives with the Mce4A: A combined spectroscopic and molecular dynamic simulation studies. International Journal of Biological Macromolecules, 2018, 111, 548-560.	3.6	45
26	Molecular interaction studies on ellagic acid for its anticancer potential targeting pyruvate dehydrogenase kinase 3. RSC Advances, 2019, 9, 23302-23315.	1.7	44
27	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.	1.8	43
28	B Cell Lymphoma 2: A Potential Therapeutic Target for Cancer Therapy. International Journal of Molecular Sciences, 2021, 22, 10442.	1.8	39
29	Identification of Sphingosine Kinase-1 Inhibitors from Bioactive Natural Products Targeting Cancer Therapy. ACS Omega, 2020, 5, 14720-14729.	1.6	38
30	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.	1.8	38
31	Identification of High-Affinity Inhibitors of Cyclin-Dependent Kinase 2 Towards Anticancer Therapy. Molecules, 2019, 24, 4589.	1.7	37
32	Discovery of Harmaline as a Potent Inhibitor of Sphingosine Kinase-1: A Chemopreventive Role in Lung Cancer. ACS Omega, 2020, 5, 21550-21560.	1.6	35
33	Investigation of deleterious effects of nsSNPs in the POT1 gene: a structural genomicsâ€based approach to understand the mechanism of cancer development. Journal of Cellular Biochemistry, 2019, 120, 10281-10294.	1.2	32
34	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.	2.0	32
35	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.	1.0	30
36	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.	2.0	29

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37	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.	1.9	26
38	Identification of Phytoconstituents as Potent Inhibitors of Casein Kinase-1 Alpha Using Virtual Screening and Molecular Dynamics Simulations. Pharmaceutics, 2021, 13, 2157.	2.0	25
39	Identification of plant-based hexokinase 2 inhibitors: combined molecular docking and dynamics simulation studies. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10319-10331.	2.0	23
40	Î²2-spectrin (SPTBN1) as a therapeutic target for diet-induced liver disease and preventing cancer development. Science Translational Medicine, 2021, 13, eabk2267.	5.8	23
41	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.	2.0	22
42	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.	1.2	20
43	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.	2.0	19
44	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.	3.6	18
45	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.	2.0	18
46	Structural genomics approach to investigate deleterious impact of nsSNPs in conserved telomere maintenance component 1. Scientific Reports, 2021, 11, 10202.	1.6	18
47	Structural and functional impact of non-synonymous SNPs in the CST complex subunit TEN1: structural genomics approach. Bioscience Reports, 2019, 39, .	1.1	17
48	Identification and structureâ€“activity relationship (SAR) studies of carvacrol derivatives as potential anti-malarial against Plasmodium falciparum falcipain-2 protease. Bioorganic Chemistry, 2020, 103, 104142.	2.0	16
49	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.	2.0	16
50	Insights into the Conserved Regulatory Mechanisms of Human and Yeast Aging. Biomolecules, 2020, 10, 882.	1.8	15
51	Bioactive phytoconstituents as potent inhibitors of casein kinase-2: dual implications in cancer and COVID-19 therapeutics. RSC Advances, 2022, 12, 7872-7882.	1.7	14
52	Design and Development of Novel Urea, Sulfonyltriurea, and Sulfonamide Derivatives as Potential Inhibitors of Sphingosine Kinase 1. Pharmaceuticals, 2020, 13, 118.	1.7	13
53	Multispectroscopic and Molecular Docking Insight into Elucidating the Interaction of Irisin with Rivastigmine Tartrate: A Combinational Therapy Approach to Fight Alzheimerâ€™s Disease. ACS Omega, 2021, 6, 7910-7921.	1.6	13
54	Investigating single amino acid substitutions in PIM1 kinase: A structural genomics approach. PLoS ONE, 2021, 16, e0258929.	1.1	13

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55	Aurora B kinase: a potential drug target for cancer therapy. Journal of Cancer Research and Clinical Oncology, 2021, 147, 2187-2198.	1.2	12
56	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.	1.0	12
57	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.	1.6	12
58	Impact of single amino acid substitution on the structure and function of TANKâ€binding kinaseâ€1. Journal of Cellular Biochemistry, 2021, 122, 1475-1490.	1.2	11
59	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.	1.4	11
60	Inhibiting Cyclin-Dependent Kinase 6 by Taurine: Implications in Anticancer Therapeutics. ACS Omega, 2022, 7, 25844-25852.	1.6	10
61	Therapeutic targeting of TANK-binding kinase signaling towards anticancer drug development: Challenges and opportunities. International Journal of Biological Macromolecules, 2022, 207, 1022-1037.	3.6	9
62	Cinnamomum zeylanicum Extract and its Bioactive Component Cinnamaldehyde Show Anti-Tumor Effects via Inhibition of Multiple Cellular Pathways. Frontiers in Pharmacology, 0, 13, .	1.6	8
63	Biophysical Insights into Implications of PEG-400 on the Î±-Crystallin Structure: Multispectroscopic and Microscopic Approach. ACS Omega, 2020, 5, 19210-19216.	1.6	7
64	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.	1.0	7
65	Structure, function and therapeutic implications of OB-fold proteins: A lesson from past to present. Briefings in Functional Genomics, 2020, 19, 377-389.	1.3	6
66	Targeting metacaspase-3 fromPlasmodium falciparumtowards antimalarial therapy: A combined approach ofin-silicoandin-vitroinvestigation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 421-430.	2.0	6
67	Comparative analysis of web-based programs for single amino acid substitutions in proteins. PLoS ONE, 2022, 17, e0267084.	1.1	6
68	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.	2.0	5
69	Modern Approaches in Synthetic Biology: Genome Editing, Quorum Sensing, and Microbiome Engineering. , 2018, , 189-205.		4
70	Impact of Single Amino Acid Substitutions in Parkinsonism-Associated Deglycase-PARK7 and Their Association with Parkinsonâ€™s Disease. Journal of Personalized Medicine, 2022, 12, 220.	1.1	4
71	Target-Based Virtual Screening of Natural Compounds Identifies a Potent Antimalarial With Selective Falcipain-2 Inhibitory Activity. Frontiers in Pharmacology, 2022, 13, 850176.	1.6	4
72	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.	1.1	3

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73	Investigating the structural features of chromodomain proteins in the human genome and predictive impacts of their mutations in cancers. International Journal of Biological Macromolecules, 2019, 131, 1101-1116.	3.6	2
74	Therapeutic Potential of Polyphenols in Alzheimerâ€™s Therapy: Broad-Spectrum and Minimal Side Effects as Key Aspects. , 2021, , 111-133.		2
75	Genome Microbiology for Synthetic Applications. , 2018, , 75-86.		1
76	Implication of Synthetic Biology in Biotherapeutic Engineering. , 2020, , 245-253.		1
77	Role of Genome-Wide Association Studies in Host Genetics: Toward Understanding of Microbiome Association. , 2020, , 37-54.		0
78	ASSESSING THE ASSESSMENT AND EVALUATION PROCESS AT PYP: A CASE STUDY. Indonesian EFL Journal, 2018, 4, 23.	0.3	0
79	Discovery of Novel Drug Targets in Microbial Pathogens Among Hypothetical Proteins: Methods and Significance. , 2019, , 377-391.		0
80	Genome Engineering Tools in Immunotherapy. , 2020, , 73-102.		0
81	Serum and glucocorticoid-regulated kinase 1: A potential target for anticancer therapy. , 2022, , 223-238.		0