Syed Sikander Azam

List of Publications by Year
in descending order

100 papers	2,010 citations	236612 25 h-index	315357 38 g-index
102 all docs	102 docs citations	102 times ranked	2237 citing authors

#	Article	IF	Citations
1	Molecular docking studies for the identification of novel melatoninergic inhibitors for acetylserotonin-O-methyltransferase using different docking routines. Theoretical Biology and Medical Modelling, 2013, 10, 63.	2.1	144
2	Binding mode analysis, dynamic simulation and binding free energy calculations of the MurF ligase from Acinetobacter baumannii. Journal of Molecular Graphics and Modelling, 2017, 77, 72-85.	1.3	84
3	Hydration of Sodium(I) and Potassium(I) Revisited: A Comparative QM/MM and QMCF MD Simulation Study of Weakly Hydrated Ions. Journal of Physical Chemistry A, 2009, 113, 1827-1834.	1.1	78
4	Benzimidazole derivatives as new Î±-glucosidase inhibitors and in silico studies. Bioorganic Chemistry, 2016, 64, 29-36.	2.0	75
5	Towards a peptide-based vaccine against Shigella sonnei : A subtractive reverse vaccinology based approach. Biologicals, 2017, 50, 87-99.	0.5	71
6	Combating tigecycline resistant Acinetobacter baumannii: A leap forward towards multi-epitope based vaccine discovery. European Journal of Pharmaceutical Sciences, 2019, 132, 1-17.	1.9	54
7	Identification of plausible drug targets by investigating the druggable genome of MDR Staphylococcus epidermidis. Gene Reports, 2017, 7, 147-153.	0.4	53
8	Molecular dynamics simulation studies of novel Î²-lactamase inhibitor. Journal of Molecular Graphics and Modelling, 2017, 74, 143-152.	1.3	53
9	Immunoinformatics characterization of SARS-CoV-2 spike glycoprotein for prioritization of epitope based multivalent peptide vaccine. Journal of Molecular Liquids, 2020, 314, 113612.	2.3	50
10	Vaccinomics to design a novel single chimeric subunit vaccine for broad-spectrum immunological applications targeting nosocomial Enterobacteriaceae pathogens. European Journal of Pharmaceutical Sciences, 2020, 146, 105258.	1.9	44
11	Binding free energy based analysis of arsenic (+ 3 oxidation state) methyltransferase with S-adenosylmethionine. Journal of Molecular Liquids, 2016, 220, 375-382.	2.3	42
12	Beryllium(II): The Strongest Structure-Forming Ion in Water? A QMCF MD Simulation Study. Journal of Physical Chemistry B, 2009, 113, 9289-9295.	1.2	39
13	Interaction mechanisms of a melatonergic inhibitor in the melatonin synthesis pathway. Journal of Molecular Liquids, 2016, 221, 507-517.	2.3	39
14	Comparative subtractive proteomics based ranking for antibiotic targets against the dirtiest superbug: Acinetobacter baumannii. Journal of Molecular Graphics and Modelling, 2018, 82, 74-92.	1.3	39
15	Selective glycosidase inhibitors: A patent review (2012â€“present). International Journal of Biological Macromolecules, 2018, 111, 82-91.	3.6	38
16	Subtractive genome analysis for in silico identification and characterization of novel drug targets in Streptococcus pneumonia strain JJA. Microbial Pathogenesis, 2018, 115, 194-198.	1.3	37
17	An insight into the exploration of druggable genome of Streptococcus gordonii for the identification of novel therapeutic candidates. Genomics, 2014, 104, 203-214.	1.3	36
18	A one-pot multicomponent facile synthesis of dihydropyrimidin-2(1H)-thione derivatives using triphenylgermane as a catalyst and its binding pattern validation. RSC Advances, 2016, 6, 79651-79661.	1.7	35

#	Article	IF	Citations
19	Design of a Novel Multi Epitope-Based Vaccine for Pandemic Coronavirus Disease (COVID-19) by Vaccinomics and Probable Prevention Strategy against Avenging Zoonotics. European Journal of Pharmaceutical Sciences, 2020, 151, 105387.	1.9	33
20	Ferrocene-based guanidine derivatives: InÂvitro antimicrobial, DNA binding and docking supported urease inhibition studies. European Journal of Medicinal Chemistry, 2014, 85, 438-449.	2.6	32
21	Immuno-informatics driven proteome-wide investigation revealed novel peptide-based vaccine targets against emerging multiple drug resistant Providencia stuartii. Journal of Molecular Graphics and Modelling, 2018, 80, 238-250.	1.3	32
22	Structure and dynamics of alpha-glucosidase through molecular dynamics simulation studies. Journal of Molecular Liquids, 2012, 174, 58-62.	2.3	31
23	Metabolic pathway analysis approach: Identification of novel therapeutic target against methicillin resistant Staphylococcus aureus. Gene, 2015, 556, 213-226.	1.0	31
24	Toward novel inhibitors against KdsB: a highly specific and selective broad-spectrum bacterial enzyme. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1326-1345.	2.0	30
25	Classical and QM/MM MD simulations of sodium(I) and potassium(I) ions in aqueous solution. Journal of Molecular Liquids, 2010, 153, 95-100.	2.3	29
26	Identification and characterization of potential druggable targets among hypothetical proteins of extensively drug resistant Mycobacterium tuberculosis (XDR KZN 605) through subtractive genomics approach. European Journal of Pharmaceutical Sciences, 2018, 114, 13-23.	1.9	28
27	Immunoinformatics design of a novel multi-epitope peptide vaccine to combat multi-drug resistant infections caused by Vibrio vulnificus. European Journal of Pharmaceutical Sciences, 2020, 142, 105160.	1.9	28
28	In silico identification of promiscuous scaffolds as potential inhibitors of 1-deoxy-<scp>d</scp>-xylulose 5-phosphate reductoisomerase for treatment of Falciparum malaria. Pharmaceutical Biology, 2017, 55, 19-32.	1.3	27
29	Subtractive Genomics, Molecular Docking and Molecular Dynamics Simulation Revealed LpxC as a Potential Drug Target Against Multi-Drug Resistant Klebsiella pneumoniae. Interdisciplinary Sciences, Computational Life Sciences, 2019, 11, 508-526.	2.2	26
30	Antiproliferative, antioxidant and binding mechanism analysis of prodigiosin from newly isolated radio-resistant Streptomyces sp. strain WMA-LM31. Molecular Biology Reports, 2018, 45, 1787-1798.	1.0	24
31	AFD: an application for bi-molecular interaction using axial frequency distribution. Journal of Molecular Modeling, 2018, 24, 84.	0.8	23
32	Molecular docking studies of potent inhibitors of tyrosinase and Î±-glucosidase. Medicinal Chemistry Research, 2012, 21, 1677-1683.	1.1	22
33	Structural investigations, anti-leishmanial, antibacterial and docking studies of new pentavalent antimony carboxylates. Inorganica Chimica Acta, 2018, 474, 148-155.	1.2	22
34	Subtractive proteomics and immunoinformatics revealed novel B-cell derived T-cell epitopes against Yersinia enterocolitica: An etiological agent of Yersiniosis. Microbial Pathogenesis, 2018, 125, 336-348.	1.3	22
35	Proteome-wide subtractive approach to prioritize a hypothetical protein of XDR-Mycobacterium tuberculosis as potential drug target. Genes and Genomics, 2019, 41, 1281-1292.	0.5	22
36	Structure and dynamics studies of sterol 24-C-methyltransferase with mechanism based inactivators for the disruption of ergosterol biosynthesis. Molecular Biology Reports, 2014, 41, 4279-4293.	1.0	21

#	Article	IF	Citations
37	A novel approach of virulome based reverse vaccinology for exploring and validating peptide-based vaccine candidates against the most troublesome nosocomial pathogen: Acinetobacter baumannii. Journal of Molecular Graphics and Modelling, 2018, 83, 1-11.	1.3	21
38	In silico screening of antigenic B-cell derived T-cell epitopes and designing of a multi-epitope peptide vaccine for Acinetobacter nosocomialis. Journal of Molecular Graphics and Modelling, 2020, 94, 107477.	1.3	20
39	Identification of putative non-host essential genes and novel drug targets against Acinetobacter baumannii by in silico comparative genome analysis. Microbial Pathogenesis, 2019, 128, 28-35.	1.3	19
40	Screening Pipeline for Flavivirus Based Inhibitors for Zika Virus NS1. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2020, 17, 1751-1761.	1.9	19
41	Discovery of beta-lactamase CMY-10 inhibitors for combination therapy against multi-drug resistant Enterobacteriaceae. PLoS ONE, 2021, 16, e0244967.	1.1	19
42	Antileishmanial, DNA Interaction, and Docking Studies of Some Ferroceneâ€Based Heteroleptic Pentavalent Antimonials. Archiv Der Pharmazie, 2016, 349, 50-62.	2.1	18
43	Synthesis, molecular docking and comparative efficacy of various alkyl/aryl thioureas as antibacterial, antifungal and Ì±-amylase inhibitors. Computational Biology and Chemistry, 2018, 77, 193-198.	1.1	18
44	Cloning and functional characterization of endo-Î²-1,4-glucanase gene from metagenomic library of vermicompost. Journal of Microbiology, 2013, 51, 329-335.	1.3	16
45	Visualizing proteinâ€“ligand binding with chemical energy-wise decomposition (CHEWD): application to ligand binding in the kallikrein-8 S1 Site. Journal of Computer-Aided Molecular Design, 2019, 33, 461-475.	1.3	16
46	Binding pattern analysis and structural insight into the inhibition mechanism of Sterol 24-C methyltransferase by docking and molecular dynamics approach. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2563-2577.	2.0	15
47	Bioactive Heteroleptic Bismuth(V) Complexes: Synthesis, Structural Analysis and Binding Pattern Validation. Applied Organometallic Chemistry, 2019, 33, e5061.	1.7	14
48	Germanium(II) in water: An unusual hydration structure results of a QMCF MD simulation. Chemical Physics Letters, 2009, 470, 85-89.	1.2	13
49	Docking and molecular dynamics simulation studies on glycation-induced conformational changes of human paraoxonase 1. European Biophysics Journal, 2012, 41, 241-248.	1.2	13
50	Identification of potent inhibitors for chromodomain-helicase- DNA-binding protein 1-like through moleculardocking studies. Medicinal Chemistry Research, 2016, 25, 2924-2939.	1.1	12
51	Identification of natural inhibitors against Acinetobacter baumannii d-alanine-d-alanine ligase enzyme: A multi-spectrum in silico approach. Journal of Molecular Liquids, 2018, 262, 460-475.	2.3	12
52	Proteome-wide identification of epitope-based vaccine candidates against multi-drug resistant Proteus mirabilis. Biologicals, 2018, 55, 27-37.	0.5	12
53	Identification of potential antibiotic targets in the proteome of multi-drug resistant Proteus mirabilis. Meta Gene, 2018, 18, 167-173.	0.3	11
54	Identification of glucosyl-3-phosphoglycerate phosphatase as a novel drug target against resistant strain of Mycobacterium tuberculosis (XDR1219) by using comparative metabolic pathway approach. Computational Biology and Chemistry, 2019, 79, 91-102.	1.1	11

#	Article	IF	Citations
55	Deciphering the Inhibition Mechanism of under Trial Hsp90 Inhibitors and Their Analogues: A Comparative Molecular Dynamics Simulation. Journal of Chemical Information and Modeling, 2020, 60, 3812-3830.	2.5	11
56	Structural and dynamical aspects of Streptococcus gordonii FabH through molecular docking and MD simulations. Journal of Molecular Graphics and Modelling, 2015, 60, 180-196.	1.3	10
57	From phylogeny to protein dynamics: A computational hierarchical quest for potent drug identification against an emerging enteropathogen â€œYersinia enterocoliticaâ€• Journal of Molecular Liquids, 2018, 265, 372-389.	2.3	10
58	Identification of unique binding site and molecular docking studies for structurally diverse Bcl-xL inhibitors. Medicinal Chemistry Research, 2014, 23, 3765-3783.	1.1	9
59	Comparative modeling and virtual screening for the identification of novel inhibitors for myo-inositol-1-phosphate synthase. Molecular Biology Reports, 2014, 41, 5039-5052.	1.0	9
60	Structural dynamics and inhibitor searching for Wnt-4 protein using comparative computational studies. Drug Design, Development and Therapy, 2015, 9, 2449.	2.0	9
61	Identification and functional characterization of novel transcriptional enhancers involved in regulating human <scp>GLI</scp>3 expression during early development. Development Growth and Differentiation, 2015, 57, 570-580.	0.6	9
62	Computational identification of potential drug targets against Mycobacterium leprae. Medicinal Chemistry Research, 2016, 25, 473-481.	1.1	9
63	Role of N-acetylserotonin O-methyltransferase in bipolar disorders and its dynamics. Journal of Molecular Liquids, 2013, 182, 25-31.	2.3	8
64	Identification of Histone Deacetylase (HDAC) as a drug target against MRSA via interolog method of protein-protein interaction prediction. European Journal of Pharmaceutical Sciences, 2017, 106, 198-211.	1.9	8
65	Subtractive proteomics revealed plausible drug candidates in the proteome of multi-drug resistant Corynebacterium diphtheriae. Meta Gene, 2018, 17, 34-42.	0.3	8
66	Structure Based in Silico Screening Revealed a Potent Acinetobacter Baumannii Ftsz Inhibitor From Asinex Antibacterial Library. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2022, 19, 3008-3018.	1.9	8
67	Role of thumb index fold in Wnt-4 protein and its dynamics through a molecular dynamics simulation study. Journal of Molecular Liquids, 2014, 198, 313-321.	2.3	7
68	The Vitality of Swivel Domain Motion in Performance of Enzyme I of Phosphotransferase System; A Comprehensive Molecular Dynamic Study. Journal of Molecular Liquids, 2017, 242, 1184-1198.	2.3	7
69	Heteroleptic copper(<scp>i</scp>) halides with triphenylphosphine and acetylthiourea: synthesis, characterization and biological studies (experimental and molecular docking). New Journal of Chemistry, 2019, 43, 19318-19330.	1.4	7
70	A combine approach of chemical synthesis, biological evaluation and structural dynamics studies revealed thiazole substituted arylamine derivatives as potent FabH enzyme inhibitors. Bioorganic Chemistry, 2020, 105, 104426.	2.0	7
71	Bioactive heteroleptic Bismuth(V) carboxylates: Synthetic Stratagem, characterization and binding pattern validation. Journal of Organometallic Chemistry, 2020, 921, 121357.	0.8	7
72	Synthesis, structural characterization, and molecular docking studies of bioactive bismuth(III) complexes with substituted hydrazones. Journal of Molecular Structure, 2021, 1230, 129870.	1.8	7

#	Article	IF	Citations
73	Hydrated germanium (II): Irregular structural and dynamical properties revealed by a quantum mechanical charge field molecular dynamics study. Journal of Computational Chemistry, 2010, 31, 278-285.	1.5	6
74	Moleculer dynamics simulaiton revealed reciever domain of Acinetobacter baumannii BfmR enzyme as the hot spot for future antibiotics designing. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2897-2912.	2.0	6
75	Genomic features of human limb specific enhancers. Genomics, 2016, 108, 143-150.	1.3	5
76	The methicillin-resistant S. epidermidis strain RP62A genome mining for potential novel drug targets identification. Gene Reports, 2017, 8, 88-93.	0.4	5
77	Inâ€vitro antileishmanial potential of peptide drug hirudin. Chemical Biology and Drug Design, 2017, 89, 67-73.	1.5	5
78	Blocking the catalytic mechanism of MurC ligase enzyme from Acinetobacter baumannii: An in Silico guided study towards the discovery of natural antibiotics. Journal of Molecular Liquids, 2019, 281, 117-133.	2.3	5
79	Immunoinformatics based designing and simulation of multi-epitope vaccine against multi-drug resistant Stenotrophomonas maltophilia. Journal of Molecular Liquids, 2021, 340, 116899.	2.3	5
80	Structure modeling and docking study of HCV NS5B-3a RNA polymerase for the identification of potent inhibitors. Medicinal Chemistry Research, 2014, 23, 618-627.	1.1	4
81	Comparative modeling and molecular docking studies of d-Alanine:d-alanine ligase: a target of antibacterial drugs. Medicinal Chemistry Research, 2014, 23, 4108-4137.	1.1	4
82	Relational dynamics obtained through simulation studies of thioredoxin reductase: From a multi-drug resistant Entamoeba histolytica. Journal of Molecular Liquids, 2020, 307, 112939.	2.3	4
83	Role of ring positioning and preferential occupation of ligand obtained through molecular dynamics simulation of peptidoglycan associated lipoprotein (Pal). Journal of Molecular Graphics and Modelling, 2020, 98, 107585.	1.3	4
84	From normal to competo-allosteric regulation: insights into the binding pattern dynamics of DSPI protein of Pseudomonas aeruginosa. Journal of Biomolecular Structure and Dynamics, 2021, 39, 538-557.	2.0	4
85	Investigation of Novel Chemical Inhibitors of Human Lysosomal Acid Lipase: Virtual Screening and Molecular Docking Studies. Combinatorial Chemistry and High Throughput Screening, 2014, 17, 473-482.	0.6	4
86	Structural characterization and antileishmanial activity of newly synthesized organo-bismuth(V) carboxylates: experimental and molecular docking studies. Journal of Biological Inorganic Chemistry, 2022, 27, 175-187.	1.1	4
87	Structure modeling and hybrid virtual screening study of Alzheimerâ€™s associated protease kallikrein 8 for the identification of novel inhibitors. Medicinal Chemistry Research, 2014, 23, 3516-3527.	1.1	3
88	Discovery of novel Glutaminase allosteric inhibitors through drug repurposing and comparative MMGB/PBSA and molecular dynamics simulation. Computers in Biology and Medicine, 2022, 146, 105669.	3.9	3
89	An integrated computational hierarchy for identification of potent inhibitors against Shikimate Kinase enzyme from Shigella sonnei , a major cause of global dysentery. Gene Reports, 2018, 11, 283-293.	0.4	2
90	Targeting isoprenoid biosynthesis pathway in Staphylococcus lugdunensis: Comparative docking and simulation studies of conventional and allosteric sites. Journal of Molecular Liquids, 2018, 269, 426-440.	2.3	2

#	Article	IF	Citations
91	From pan-genome to protein dynamics: A computational hierarchical quest to identify drug target in multi-drug resistant Burkholderia cepacia. Journal of Molecular Liquids, 2020, 317, 113904.	2.3	2
92	Structural Characterization of Alpha-methylacyl-CoA Racemase: Comparative Structural Modeling, Molecular Docking and Dynamic Simulations Studies. Current Cancer Drug Targets, 2015, 15, 822-835.	0.8	2
93	Insight into natural inhibitors and bridging docking to dynamic simulation against sugar Isomerase (SIS) domain protein. Journal of Molecular Modeling, 2020, 26, 221.	0.8	1
94	Conformational transition of Acinetobacter baumannii KdsC enzyme and the role of magnesium in binding: An insight from comparative molecular dynamics simulation and its implications in novel antibiotics design. Journal of Molecular Graphics and Modelling, 2020, 99, 107625.	1.3	1
95	A computational subtractive genome analysis for the characterization of novel drug targets in Klebsiella pneumonia strain PittNDM01. Microbial Pathogenesis, 2020, 146, 104245.	1.3	1
96	Senna makki and other active phytochemicals: Myths and realities behind covid19 therapeutic interventions. PLoS ONE, 2022, 17, e0268454.	1.1	1
97	Distribution of biological databases over low-bandwidth networks. Bioinformation, 2012, 8, 239-242.	0.2	0
98	Structure and dynamic studies of lunatic, manic and radical fringe. Journal of Molecular Liquids, 2013, 188, 186-195.	2.3	0
99	Deciphering the role of sulfonamides and molecular basis of thioredoxin domain dynamics through comparative simulations. Journal of Molecular Liquids, 2021, 321, 114797.	2.3	0
100	Structure-based Virtual Screening Approach for the Discovery of Potent Inhibitors of Aminoglycoside 6'-N-Acetyltransferase Type Ib [AAC(6')-Ib] against K. pneumoniae Infections. Letters in Drug Design and Discovery, 2020, 17, 1027-1035.	0.4	0