Syed Sikander Azam

List of Publications by Year
in descending order

100	2,010	236612	315357
papers	citations	25 h-index	38 g-index

102	102	102	2237
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	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
3	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
4	Senna makki and other active phytochemicals: Myths and realities behind covid19 therapeutic interventions. PLoS ONE, 2022, 17, e0268454.	1.1	1
5	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
6	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
7	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
8	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
9	Discovery of beta-lactamase CMY-10 inhibitors for combination therapy against multi-drug resistant Enterobacteriaceae. PLoS ONE, 2021, 16, e0244967.	1.1	19
10	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
11	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
12	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
13	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
14	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
15	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
16	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
17	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
18	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

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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	Bioactive heteroleptic Bismuth(V) carboxylates: Synthetic Stratagem, characterization and binding pattern validation. Journal of Organometallic Chemistry, 2020, 921, 121357.	0.8	7
21	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
22	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
23	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
24	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
25	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
26	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
27	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
28	Bioactive Heteroleptic Bismuth(V) Complexes: Synthesis, Structural Analysis and Binding Pattern Validation. Applied Organometallic Chemistry, 2019, 33, e5061.	1.7	14
29	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
30	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
31	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
32	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
33	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
34	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
35	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
36	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

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37	AFD: an application for bi-molecular interaction using axial frequency distribution. Journal of Molecular Modeling, 2018, 24, 84.	0.8	23
38	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
39	Subtractive proteomics revealed plausible drug candidates in the proteome of multi-drug resistant Corynebacterium diphtheriae. Meta Gene, 2018, 17, 34-42.	0.3	8
40	Structural investigations, anti-leishmanial, antibacterial and docking studies of new pentavalent antimony carboxylates. Inorganica Chimica Acta, 2018, 474, 148-155.	1.2	22
41	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
42	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
43	Selective glycosidase inhibitors: A patent review (2012â€“present). International Journal of Biological Macromolecules, 2018, 111, 82-91.	3.6	38
44	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
45	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
46	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
47	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
48	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
49	Synthesis, molecular docking and comparative efficacy of various alkyl/aryl thioureas as antibacterial, antifungal and l±-amylase inhibitors. Computational Biology and Chemistry, 2018, 77, 193-198.	1.1	18
50	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
51	Identification of potential antibiotic targets in the proteome of multi-drug resistant Proteus mirabilis. Meta Gene, 2018, 18, 167-173.	0.3	11
52	Proteome-wide identification of epitope-based vaccine candidates against multi-drug resistant Proteus mirabilis. Biologicals, 2018, 55, 27-37.	0.5	12
53	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
54	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

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55	Identification of plausible drug targets by investigating the druggable genome of MDR Staphylococcus epidermidis. Gene Reports, 2017, 7, 147-153.	0.4	53
56	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
57	Molecular dynamics simulation studies of novel Î²-lactamase inhibitor. Journal of Molecular Graphics and Modelling, 2017, 74, 143-152.	1.3	53
58	Towards a peptide-based vaccine against Shigella sonnei : A subtractive reverse vaccinology based approach. Biologicals, 2017, 50, 87-99.	0.5	71
59	The methicillin-resistant S. epidermidis strain RP62A genome mining for potential novel drug targets identification. Gene Reports, 2017, 8, 88-93.	0.4	5
60	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
61	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
62	Inâ€vitro antileishmanial potential of peptide drug hirudin. Chemical Biology and Drug Design, 2017, 89, 67-73.	1.5	5
63	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
64	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
65	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
66	Antileishmanial, DNA Interaction, and Docking Studies of Some Ferroceneâ€Based Heteroleptic Pentavalent Antimonials. Archiv Der Pharmazie, 2016, 349, 50-62.	2.1	18
67	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
68	Genomic features of human limb specific enhancers. Genomics, 2016, 108, 143-150.	1.3	5
69	Interaction mechanisms of a melatonergic inhibitor in the melatonin synthesis pathway. Journal of Molecular Liquids, 2016, 221, 507-517.	2.3	39
70	Computational identification of potential drug targets against Mycobacterium leprae. Medicinal Chemistry Research, 2016, 25, 473-481.	1.1	9
71	Benzimidazole derivatives as new Î±-glucosidase inhibitors and in silico studies. Bioorganic Chemistry, 2016, 64, 29-36.	2.0	75
72	Structural dynamics and inhibitor searching for Wnt-4 protein using comparative computational studies. Drug Design, Development and Therapy, 2015, 9, 2449.	2.0	9

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73	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
74	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
75	Metabolic pathway analysis approach: Identification of novel therapeutic target against methicillin resistant Staphylococcus aureus. Gene, 2015, 556, 213-226.	1.0	31
76	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
77	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
78	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
79	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
80	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
81	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
82	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
83	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
84	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
85	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
86	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
87	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
88	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
89	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
90	Structure and dynamic studies of lunatic, manic and radical fringe. Journal of Molecular Liquids, 2013, 188, 186-195.	2.3	0

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91	Role of N-acetylserotonin O-methyltransferase in bipolar disorders and its dynamics. Journal of Molecular Liquids, 2013, 182, 25-31.	2.3	8
92	Structure and dynamics of alpha-glucosidase through molecular dynamics simulation studies. Journal of Molecular Liquids, 2012, 174, 58-62.	2.3	31
93	Distribution of biological databases over low-bandwidth networks. Bioinformation, 2012, 8, 239-242.	0.2	0
94	Molecular docking studies of potent inhibitors of tyrosinase and Î±-glucosidase. Medicinal Chemistry Research, 2012, 21, 1677-1683.	1.1	22
95	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
96	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
97	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
98	Germanium(II) in water: An unusual hydration structure results of a QMCF MD simulation. Chemical Physics Letters, 2009, 470, 85-89.	1.2	13
99	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
100	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