Sumera Zaib

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6913899/publications.pdf

Version: 2024-02-01

103	1,763	304743	377865
papers	citations	22 h-index	34 g-index

107	107	107	1874
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Synthesis, crystal structure and biological evaluation of some novel 1,2,4-triazolo[3,4-b]-1,3,4-thiadiazoles and 1,2,4-triazolo[3,4-b]-1,3,4-thiadiazines. European Journal of Medicinal Chemistry, 2014, 78, 167-177.	5.5	86
2	Synthesis, urease inhibition, antioxidant and antibacterial studies of some 4-amino-5-aryl-3H-1,2,4-triazole-3-thiones and their 3,6-disubstituted 1,2,4-triazolo[3,4-b]1,3,4-thiadiazole derivatives. Journal of the Brazilian Chemical Society, 2012, 23, 854-860.	0.6	71
3	Synthesis, characterization, and anticancer activity of Schiff bases. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3246-3259.	3.5	68
4	Active compounds from a diverse library of triazolothiadiazole and triazolothiadiazine scaffolds: Synthesis, crystal structure determination, cytotoxicity, cholinesterase inhibitory activity, and binding mode analysis. Bioorganic and Medicinal Chemistry, 2014, 22, 6163-6173.	3.0	54
5	A multi-target therapeutic potential of Prunus domestica gum stabilized nanoparticles exhibited prospective anticancer, antibacterial, urease-inhibition, anti-inflammatory and analgesic properties.. BMC Complementary and Alternative Medicine, 2017, 17, 276.	3.7	53
6	Role of Mitochondrial Membrane Potential and Lactate Dehydrogenase A in Apoptosis. Anti-Cancer Agents in Medicinal Chemistry, 2022, 22, 2048-2062.	1.7	50
7	A new entry into the portfolio of Î±-glucosidase inhibitors as potent therapeutics for type 2 diabetes: Design, bioevaluation and one-pot multi-component synthesis of diamine-bridged coumarinyl oxadiazole conjugates. Bioorganic Chemistry, 2018, 77, 190-202.	4.1	48
8	Recent advances with alkaline phosphatase isoenzymes and their inhibitors. Archiv Der Pharmazie, 2020, 353, e2000011.	4.1	48
9	Synthesis, molecular docking studies, and in vitro screening of sulfanilamide-thiourea hybrids as antimicrobial and urease inhibitors. Medicinal Chemistry Research, 2013, 22, 3653-3662.	2.4	46
10	Exploration of a library of triazolothiadiazole and triazolothiadiazine compounds as a highly potent and selective family of cholinesterase and monoamine oxidase inhibitors: design, synthesis, X-ray diffraction analysis and molecular docking studies. RSC Advances, 2015, 5, 21249-21267.	3.6	45
11	Synthesis, characterization and urease inhibition, in vitro anticancer and antileishmanial studies of Ni(II) complexes with N,N,Nâ€²-trisubstituted thioureas. Journal of Biological Inorganic Chemistry, 2015, 20, 541-554.	2.6	45
12	Didymin, a dietary citrus flavonoid exhibits anti-diabetic complications and promotes glucose uptake through the activation of PI3K/Akt signaling pathway in insulin-resistant HepG2 cells. Chemico-Biological Interactions, 2019, 305, 180-194.	4.0	44
13	New frontiers in the transition-metal-free synthesis of heterocycles from alkynoates: an overview and current status. Organic Chemistry Frontiers, 2020, 7, 3734-3791.	4.5	43
14	Solution-phase microwave assisted parallel synthesis, biological evaluation and in silico docking studies of N,Nâ€²-disubstituted thioureas derived from 3-chlorobenzoic acid. Bioorganic and Medicinal Chemistry, 2016, 24, 4452-4463.	3.0	31
15	Design of a novel multiple epitope-based vaccine: An immunoinformatics approach to combat SARS-CoV-2 strains. Journal of Infection and Public Health, 2021, 14, 938-946.	4.1	31
16	Utilization of the common functional groups in bioactive molecules: Exploring dual inhibitory potential and computational analysis of keto esters against Î±-glucosidase and carbonic anhydrase-II enzymes. International Journal of Biological Macromolecules, 2021, 167, 233-244.	7.5	30
17	Unraveling the Alkaline Phosphatase Inhibition, Anticancer, and Antileishmanial Potential of Coumarinâ€“Triazolothiadiazine Hybrids: Design, Synthesis, and Molecular Docking Analysis. Archiv Der Pharmazie, 2016, 349, 553-565.	4.1	29
18	A domino reaction of 3-chlorochromones with aminoheterocycles. Synthesis of pyrazolopyridines and benzofuropyridines and their optical and ecto-5â€²-nucleotidase inhibitory effects. Organic and Biomolecular Chemistry, 2018, 16, 717-732.	2.8	28

#	Article	IF	Citations
19	New prospects for the development of selective inhibitors of Î± -glucosidase based on coumarin-iminothiazolidinone hybrids: Synthesis, in-vitro biological screening and molecular docking analysis. Journal of the Taiwan Institute of Chemical Engineers, 2017, 81, 119-133.	5.3	26
20	Synthesis, monoamine oxidase inhibition activity and molecular docking studies of novel 4-hydroxy-Nâ€²-[benzylidene or 1-phenylethylidene]-2-H/methyl/benzyl-1,2-benzothiazine-3-carbohydrazide 1,1-dioxides. European Journal of Medicinal Chemistry, 2018, 143, 1373-1386.	5.5	26
21	Antidiabetic activities of chloroform fraction of Anthocleista vogelii Planch root bark in rats with diet- and alloxan-induced obesity-diabetes. Journal of Ethnopharmacology, 2019, 229, 293-302.	4.1	25
22	Synthesis, biological evaluation, and docking studies of new raloxifene sulfonate or sulfamate derivatives as inhibitors of nucleotide pyrophosphatase/phosphodiesterase. European Journal of Medicinal Chemistry, 2019, 181, 111560.	5.5	24
23	Hybrid Quinoline-Thiosemicarbazone Therapeutics as a New Treatment Opportunity for Alzheimerâ€™s Diseaseâ€’Synthesis, In Vitro Cholinesterase Inhibitory Potential and Computational Modeling Analysis. Molecules, 2021, 26, 6573.	3.8	24
24	Synthesis and in vitro Bio-activity Evaluation of N4-benzyl Substituted 5-Chloroisatin-3-thiosemicarbazones as Urease and Glycation Inhibitors. Acta Chimica Slovenica, 2018, 65, 108-118.	0.6	23
25	Synthesis and in vitro urease inhibitory activity of benzohydrazide derivatives, in silico and kinetic studies. Bioorganic Chemistry, 2019, 82, 163-177.	4.1	22
26	Synthesis, molecular modelling and biological evaluation of tetrasubstituted thiazoles towards cholinesterase enzymes and cytotoxicity studies. Bioorganic Chemistry, 2018, 78, 141-148.	4.1	21
27	Histone Modifications and their Role in Epigenetics of Cancer. Current Medicinal Chemistry, 2022, 29, 2399-2411.	2.4	21
28	Exploiting the potential of aryl acetamide derived Zn(<scp>ii</scp>) complexes in medicinal chemistry: synthesis, structural analysis, assessment of biological profile and molecular docking studies. New Journal of Chemistry, 2016, 40, 7084-7094.	2.8	20
29	Synthesis, crystal structure, molecular docking studies and bio-evaluation of some N ⁴-benzyl-substituted isatin- 3-thiosemicarbazones as urease and glycation inhibitors. Heterocyclic Communications, 2018, 24, 51-58.	1.2	20
30	Carbonic anhydrase inhibition of Schiff base derivative of imino-methyl-naphthalen-2-ol: Synthesis, structure elucidation, molecular docking, dynamic simulation and density functional theory calculations. Journal of Molecular Structure, 2018, 1156, 193-200.	3.6	20
31	Synthesis, biological evaluation, and docking studies of new pyrazole-based thiourea and sulfonamide derivatives as inhibitors of nucleotide pyrophosphatase/phosphodiesterase. Bioorganic Chemistry, 2020, 99, 103783.	4.1	20
32	Investigation of potent inhibitors of cholinesterase based on thiourea and pyrazoline derivatives: Synthesis, inhibition assay and molecular modeling studies. Bioorganic Chemistry, 2019, 90, 103036.	4.1	19
33	Potent Inhibitors of Cholinesterases: A Biochemical and In Silico Approach. Molecules, 2021, 26, 656.	3.8	19
34	Synthesis, biological evaluation and docking studies of some novel isatin-3-hydrazonothiazolines. RSC Advances, 2016, 6, 60826-60844.	3.6	18
35	Pyrazolobenzothiazine-based carbothioamides as new structural leads for the inhibition of monoamine oxidases: design, synthesis, in vitro bioevaluation and molecular docking studies. MedChemComm, 2017, 8, 452-464.	3.4	18
36	Exploration of aroyl/heteroaroyl iminothiazolines featuring 2,4,5-trichlorophenyl moiety as a new class of potent, selective, and in vitro efficacious glucosidase inhibitors. Bioorganic Chemistry, 2017, 74, 134-144.	4.1	18

#	Article	IF	Citations
37	Design, synthesis and biological evaluation of trinary benzocoumarin-thiazoles-azomethines derivatives as effective and selective inhibitors of alkaline phosphatase. Bioorganic Chemistry, 2019, 91, 103137.	4.1	18
38	Synthetic and medicinal chemistry of phthalazines: Recent developments, opportunities and challenges. Bioorganic Chemistry, 2020, 105, 104425.	4.1	18
39	Symmetrical aryl linked bis-iminothiazolidinones as new chemical entities for the inhibition of monoamine oxidases: Synthesis, in vitro biological evaluation and molecular modelling analysis. Bioorganic Chemistry, 2017, 70, 17-26.	4.1	17
40	Synthesis, biological evaluation, and molecular docking study of sulfonate derivatives as nucleotide pyrophosphatase/phosphodiesterase (NPP) inhibitors. Bioorganic and Medicinal Chemistry, 2019, 27, 2741-2752.	3.0	17
41	Investigation of new quinoline derivatives as promising inhibitors of NTPDases: Synthesis, SAR analysis and molecular docking studies. Bioorganic Chemistry, 2019, 87, 218-226.	4.1	17
42	Synthesis, characterization, in vitro tissue-nonspecific alkaline phosphatase (TNAP) and intestinal alkaline phosphatase (IAP) inhibition studies and computational evaluation of novel thiazole derivatives. Bioorganic Chemistry, 2020, 102, 104088.	4.1	17
43	New acetylphenol-based acyl thioureas broaden the scope of drug candidates for urease inhibition: synthesis, in vitro screening and in silico analysis. International Journal of Biological Macromolecules, 2022, 198, 157-167.	7.5	17
44	Pd(II)-based heteroleptic complexes with N-(acyl)-Nâ€², Nâ€²-(disubstituted)thioureas and phosphine ligands: Synthesis, characterization and cytotoxic studies against lung squamous, breast adenocarcinoma and Leishmania tropica. Inorganica Chimica Acta, 2018, 479, 189-196.	2.4	16
45	Alkynoates as Versatile and Powerful Chemical Tools for the Rapid Assembly of Diverse Heterocycles under Transition-Metal Catalysis: Recent Developments and Challenges. Topics in Current Chemistry, 2021, 379, 3.	5.8	16
46	Preparation, Characterization, and Pharmacological Investigation of Withaferin-A Loaded Nanosponges for Cancer Therapy; In Vitro, In Vivo and Molecular Docking Studies. Molecules, 2021, 26, 6990.	3.8	16
47	Synthesis, characterization, monoamine oxidase inhibition, molecular docking and dynamic simulations of novel 2,1-benzothiazine-2,2-dioxide derivatives. Bioorganic Chemistry, 2018, 80, 498-510.	4.1	15
48	Quinolinic Carboxylic Acid Derivatives as Potential Multi-target Compounds for Neurodegeneration: Monoamine Oxidase and Cholinesterase Inhibition. Medicinal Chemistry, 2018, 14, 74-85.	1.5	15
49	Synthesis, X-ray crystal and monoamine oxidase inhibitory activity of 4,6-dihydrobenzo[c]pyrano[2,3-e][1,2]thiazine 5,5-dioxides: In vitro studies and docking analysis. European Journal of Pharmaceutical Sciences, 2019, 131, 9-22.	4.0	14
50	Poncirin, an orally active flavonoid exerts antidiabetic complications and improves glucose uptake activating PI3K/Akt signaling pathway in insulin resistant C2C12 cells with anti-glycation capacities. Bioorganic Chemistry, 2020, 102, 104061.	4.1	14
51	Dithallium(III)-Containing 30-Tungsto-4-phosphate, [Tl₂Na₂(H₂O)₂(P₂W₁₅O₅₆)₂]¹⁶⁻: Synthesis, Structural Characterization, and Biological Studies. Inorganic Chemistry, 2018, 57, 7168-7179.	4.1	13
52	Discovery of urease inhibitory effect of sulfamate derivatives: Biological and computational studies. Bioorganic Chemistry, 2022, 119, 105545.	4.1	12
53	Synthesis, X-ray molecular structure, biological evaluation and molecular docking studies of some N 4 -benzyl substituted 5-nitroisatin-3-thiosemicarbazones. Bioorganic and Medicinal Chemistry, 2017, 25, 1022-1029.	3.0	11
54	Solution-phase microwave assisted parallel synthesis, biological evaluation and in silico docking studies of 2-chlorobenzoyl thioureas derivatives. Journal of Molecular Structure, 2018, 1164, 354-362.	3.6	11

#	Article	IF	Citations
55	Probing the high potency of pyrazolyl pyrimidinetriones and thioxopyrimidinediones as selective and efficient non-nucleotide inhibitors of recombinant human ectonucleotidases. Bioorganic Chemistry, 2019, 88, 102893.	4.1	11
56	Synthesis, characterization, alkaline phosphatase inhibition assay and molecular modeling studies of 1-benzylidene-2-(4-tert- butylthiazol-2-yl) hydrazines. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6140-6153.	3.5	11
57	Rhodanine-3-acetamide derivatives as aldose and aldehyde reductase inhibitors to treat diabetic complications: synthesis, biological evaluation, molecular docking and simulation studies. BMC Chemistry, 2021, 15, 28.	3.8	11
58	Sulfonate and sulfamate derivatives possessing benzofuran or benzothiophene nucleus as potent carbonic anhydrase II/IX/XII inhibitors. Bioorganic and Medicinal Chemistry, 2019, 27, 3889-3901.	3.0	10
59	Exploiting oxadiazole-sulfonamide hybrids as new structural leads to combat diabetic complications via aldose reductase inhibition. Bioorganic Chemistry, 2020, 99, 103852.	4.1	10
60	Inhibition of Angiotensin-I Converting Enzyme by Ginsenosides: Structureâ€“Activity Relationships and Inhibitory Mechanism. Journal of Agricultural and Food Chemistry, 2021, 69, 6073-6086.	5.2	10
61	CRISPR-Cas9 Genome Engineering: Trends in Medicine and Health. Mini-Reviews in Medicinal Chemistry, 2022, 22, 410-421.	2.4	10
62	Evaluation of sulfonate and sulfamate derivatives possessing benzofuran or benzothiophene nucleus as inhibitors of nucleotide pyrophosphatases/phosphodiesterases and anticancer agents. Bioorganic Chemistry, 2020, 104, 104305.	4.1	9
63	Bisthioureas of pimelic acid and 4-methylsalicylic acid derivatives as selective inhibitors of tissue-nonspecific alkaline phosphatase (TNAP) and intestinal alkaline phosphatase (IAP): Synthesis and molecular docking studies. Bioorganic Chemistry, 2020, 101, 103996.	4.1	9
64	Antidiabetic potential of methanol extracts from leaves of Piper umbellatum L. and Persea americana Mill.. Asian Pacific Journal of Tropical Biomedicine, 2018, 8, 160.	1.2	9
65	Fabrication and Biological Assessment of Antidiabetic Î±-Mangostin Loaded Nanosponges: In Vitro, In Vivo, and In Silico Studies. Molecules, 2021, 26, 6633.	3.8	9
66	An efficient numerical simulation and mathematical modeling for the prevention of tuberculosis. International Journal of Biomathematics, 2022, 15, .	2.9	9
67	Fabrication and Evaluation of Voriconazole Loaded Transethosomal Gel for Enhanced Antifungal and Antileishmanial Activity. Molecules, 2022, 27, 3347.	3.8	9
68	Modification of Bischler-MÃ¶hlau indole derivatives through palladium catalyzed Suzuki reaction as effective cholinesterase inhibitors, their kinetic and molecular docking studies. Bioorganic Chemistry, 2018, 76, 166-176.	4.1	8
69	Triorganotin (IV) carboxylates as potential anticancer agents: Their synthesis, physiochemical characterization, and cytotoxic activity against HeLa and MCFâ€7 cancer cells. Applied Organometallic Chemistry, 2021, 35, e6165.	3.5	8
70	Inhibition of Aldose Reductase by Ginsenoside Derivatives via a Specific Structure Activity Relationship with Kinetics Mechanism and Molecular Docking Study. Molecules, 2022, 27, 2134.	3.8	8
71	Structure-based virtual screening of dipeptidyl peptidase 4 inhibitors and their in vitro analysis. Computational Biology and Chemistry, 2021, 91, 107326.	2.3	7
72	An efficient synthetic approach toward a sporadic heterocyclic scaffold: 1,3-Oxathiol-2-ylidenes; alkaline phosphatase inhibition and molecular docking studies. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127238.	2.2	7

#	Article	IF	Citations
73	Cytotoxicity, Pro-apoptotic Activity and in silico Studies of Dithiocarbamates and their Structure Based Design and SAR Studies. Medicinal Chemistry, 2019, 15, 892-902.	1.5	7
74	Carbonic Anhydrase Inhibitory Potential of 1,2,4-triazole-3-thione Derivatives of Flurbiprofen, Ibuprofen and 4-tert-butylbenzoic Hydrazide: Design, Synthesis, Characterization, Biochemical Evaluation, Molecular Docking and Dynamic Simulation Studies. Medicinal Chemistry, 2019, 15, 298-310.	1.5	7
75	Anticancer evaluation of a manganese complex on HeLa and MCF-7 cancer cells: design, deterministic solvothermal synthesis approach, Hirshfeld analysis, DNA binding, intracellular reactive oxygen species production, electrochemical characterization and density functional theory. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1068-1081.	3.5	6
76	15-LOX Inhibitors: Biochemical Evaluation of Flurbiprofen and its Derivatives. Life and Science, 2020, 1, 6.	0.1	6
77	Investigation of solid state architectures in tetrazolyl tryptophol stabilized by crucial aromatic interactions and hydrogen bonding: Experimental and theoretical analysis. Journal of Molecular Structure, 2022, 1262, 133079.	3.6	6
78	Recent Advances in the Sustainable Synthesis of Quinazolines Using Earth-Abundant First Row Transition Metals. Current Organic Chemistry, 2020, 24, 1775-1792.	1.6	5
79	Synthesis and antitumor activities of novel Mannich base derivatives derived from natural flavonoids. , 2021, , .		5
80	Centroidâ‹¯centroid and hydrogen bond interactions as robust supramolecular units for crystal engineering: X-ray crystallographic, computational and urease inhibitory investigations of 1,2,4-triazolo[3,4-a]phthalazines. CrystEngComm, 0, , .	2.6	5
81	Synthesis and Inhibitory Activity towards Monoamine Oxidase A and B of 8â€Functionalized 3â€Fluoroâ€2â€•methylâ€benzo[4,5]thiazolo[3,2â€•a]pyrimidinâ€4â€ones. ChemistrySelect, 2019, 4, 7284-7291.	1.5	4
82	Indane-1,3-diones: As Potential and Selective Î±-glucosidase Inhibitors, their Synthesis, in vitro and in silico Studies. Medicinal Chemistry, 2021, 17, 887-902.	1.5	4
83	Synthesis, Characterization and Biological Activities of Creatinine Amides and Creatinine Schiff Bases. Medicinal Chemistry, 2017, 13, 196-203.	1.5	4
84	Highly Potent and Selective Ectonucleoside Triphosphate Diphosphohydrolase (ENTPDase1, 2, 3 and 8) Inhibitors Having 2-substituted-7- trifluoromethyl-thiadiazolopyrimidones Scaffold. Medicinal Chemistry, 2020, 16, 689-702.	1.5	4
85	Synthesis of 2â€Arylâ€12 H â€benzothiazolo[2,3â€•b]quinazolinâ€12â€•ones and Their Activity Against Monoamine Oxidases. ChemistrySelect, 2019, 4, 11071-11076.	1.5	3
86	Synthesis of 2â€Alkynylâ€•and2â€Aminoâ€12 H â€benzothiazolo[2,3â€•b]quinazolinâ€12â€•ones and Their Inhibitory Potential against Monoamine Oxidase A and B. ChemistrySelect, 2019, 4, 13760-13767.	1.5	3
87	Mechanistic insight of DACH1 receptor in the development of carcinoma insurgence through MD simulation studies. Journal of Biomolecular Structure and Dynamics, 2020, , 1-10.	3.5	3
88	Antiproliferative and Pro-Apoptotic Effects of Thiazolo[3,2â€“b][1,2,4]triazoles in Breast and Cervical Cancer Cells. Anti-Cancer Agents in Medicinal Chemistry, 2021, 21, 2181-2191.	1.7	3
89	New Hybrid Scaffolds Based on Carbazole-Chalcones as Potent Anticancer Agents. Anti-Cancer Agents in Medicinal Chemistry, 2021, 21, 1082-1091.	1.7	3
90	Synthesis of Novel Benzothiazolo[3,2â€•a]pyridimidinâ€4â€•ones with Potential Cytotoxic and Proâ€Apoptotic Potential. ChemistrySelect, 2018, 3, 12213-12218.	1.5	2

#	Article	IF	Citations
91	Sesquiterpene Coumarins from Ferula narthex 15-LOX, Î±-Glucosidase Inhibition and Molecular Docking Studies. Revista Brasileira De Farmacognosia, 2020, 30, 12-17.	1.4	2
92	Machine Intelligence Techniques for the Identification and Diagnosis of COVID-19. Current Medicinal Chemistry, 2021, 28, 5268-5283.	2.4	2
93	Nanomedicines Targeting Heat Shock Protein 90 Gene Expression in the Therapy of Breast Cancer. ChemistrySelect, 2022, 7, .	1.5	2
94	Identification of New Chromenone Derivatives as Cholinesterase Inhibitors and Molecular Docking Studies. Medicinal Chemistry, 2018, 14, 809-817.	1.5	1
95	Synthesis of Chalcones as Potential Î± â€Glucosidase Inhibitors, Inâ€Vitro and Inâ€Silico Studies. ChemistrySelect, 2021, 6, 9933-9940.	1.5	1
96	Cytotoxicity Potential of Nelsonia canescens (Lam.) Spreng Extracts against Cervical Cancer Cell Lines. Saudi Journal of Biomedical Research, 2019, 04, 439-443.	0.2	1
97	Antiproliferative and Proapoptotic Effect of Daucus carota in Cervical Cancer Cells: An In Vitro Approach. ChemistrySelect, 2022, 7, .	1.5	1
98	Preventive and Therapeutic Features of Combination Therapy for HIV. Frontiers in Clinical Drug Research - HIV, 2021, , 175-202.	0.0	0
99	In vitro Antiobesity Activities and In vivo Anti-Lipolytic Effect of Alstonia boonei Stem Bark Fraction. Proceedings for Annual Meeting of the Japanese Pharmacological Society, 2018, WCP2018, PO4-8-3.	0.0	0
100	Green Strategies for Sustainable Câ€“H Bond Functionalizations. Current Organic Chemistry, 2021, 25, 2909-2911.	1.6	0
101	Isolation and Characterization of a Flavonoid and a Neolignan from Silybum marianum : Inâ€vitro Cytotoxic Evaluation. ChemistrySelect, 2022, 7, .	1.5	0
102	Evaluation of indole-picolinamide hybrid molecules as carbonic anhydrase-II inhibitors: Biological and computational studies. Journal of Molecular Structure, 2022, , 133048.	3.6	0
103	Rational Design of Antiâ€Epileptic Peptides to Inhibit MAPK/MKPâ€2 Interactions for Epilepsy Therapeutics**. ChemistrySelect, 2022, 7, .	1.5	0