Abdul Wadood

List of Publications by Year
in descending order

169 papers	4,794 citations	81743 39 h-index	149479 56 g-index
171 all docs	171 docs citations	171 times ranked	4177 citing authors

#	Article	IF	Citations
1	Anti-Alzheimerâ€™s Studies on Î²-Sitosterol Isolated from Polygonum hydropiper L.. Frontiers in Pharmacology, 2017, 8, 697.	1.6	159
2	Isatin based Schiff bases as inhibitors of Î±-glucosidase: Synthesis, characterization, in vitro evaluation and molecular docking studies. Bioorganic Chemistry, 2015, 60, 42-48.	2.0	147
3	Synthesis and molecular docking studies of potent Î±-glucosidase inhibitors based on biscoumarin skeleton. European Journal of Medicinal Chemistry, 2014, 81, 245-252.	2.6	128
4	Triazinoindole analogs as potent inhibitors of Î±-glucosidase: Synthesis, biological evaluation and molecular docking studies. Bioorganic Chemistry, 2015, 58, 81-87.	2.0	126
5	Synthesis, molecular docking, acetylcholinesterase and butyrylcholinesterase inhibitory potential of thiazole analogs as new inhibitors for Alzheimer disease. Bioorganic Chemistry, 2015, 62, 106-116.	2.0	114
6	Antimicrobial Activity of Some Novel Armed Thiophene Derivatives and Petra/Osiris/Molinspiration (POM) Analyses. Molecules, 2016, 21, 222.	1.7	86
7	Synthesis of 4-thiazolidinone analogs as potent in vitro anti-urease agents. Bioorganic Chemistry, 2015, 63, 123-131.	2.0	85
8	Syntheses of new 3-thiazolyl coumarin derivatives, inÂvitro Î± -glucosidase inhibitory activity, and molecular modeling studies. European Journal of Medicinal Chemistry, 2016, 122, 196-204.	2.6	78
9	Synthesis of benzotriazoles derivatives and their dual potential as Î±-amylase and Î±-glucosidase inhibitors inÂvitro: Structure-activity relationship, molecular docking, and kinetic studies. European Journal of Medicinal Chemistry, 2019, 183, 111677.	2.6	78
10	5-Bromo-2-aryl benzimidazole derivatives as non-cytotoxic potential dual inhibitors of Î± -glucosidase and urease enzymes. Bioorganic Chemistry, 2017, 72, 21-31.	2.0	75
11	Synthesis of 1H-1,2,3-triazole derivatives as new Î±-glucosidase inhibitors and their molecular docking studies. Bioorganic Chemistry, 2018, 81, 98-106.	2.0	75
12	Synthesis, molecular docking and Î±-glucosidase inhibition of 5-aryl-2-(6â€²-nitrobenzofuran-2â€²-yl)-1,3,4-oxadiazoles. Bioorganic Chemistry, 2016, 66, 117-123.	2.0	71
13	New Hybrid Hydrazinyl Thiazole Substituted Chromones: As Potential Î±-Amylase Inhibitors and Radical (DPPH & ABTS) Scavengers. Scientific Reports, 2017, 7, 16980.	1.6	70
14	Synthesis, Î²-glucuronidase inhibition and molecular docking studies of hybrid bisindole-thiosemicarbazides analogs. Bioorganic Chemistry, 2016, 68, 56-63.	2.0	66
15	Hydrazinyl arylthiazole based pyridine scaffolds: Synthesis, structural characterization, inÂvitro Î±-glucosidase inhibitory activity, and in silico studies. European Journal of Medicinal Chemistry, 2017, 138, 255-272.	2.6	65
16	Synthesis, in vitro Î±-glucosidase inhibitory potential and molecular docking study of thiadiazole analogs. Bioorganic Chemistry, 2018, 78, 201-209.	2.0	65
17	Novel 2,5-disubtituted-1,3,4-oxadiazoles with benzimidazole backbone: A new class of Î²-glucuronidase inhibitors and in silico studies. Bioorganic and Medicinal Chemistry, 2015, 23, 3119-3125.	1.4	60
18	Novel quinoline derivatives as potent in vitro Î±-glucosidase inhibitors: in silico studies and SAR predictions. MedChemComm, 2015, 6, 1826-1836.	3.5	58

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19	Antioxidant and anticholinesterase potential of diterpenoid alkaloids from Aconitum heterophyllum. Bioorganic and Medicinal Chemistry, 2017, 25, 3368-3376.	1.4	55
20	Synthesis of benzothiazole derivatives as a potent Î±-glucosidase inhibitor. Bioorganic Chemistry, 2019, 85, 33-48.	2.0	54
21	Oxindole based oxadiazole hybrid analogs: Novel Î± -glucosidase inhibitors. Bioorganic Chemistry, 2018, 76, 273-280.	2.0	53
22	In vitro cholinesterase enzymes inhibitory potential and in silico molecular docking studies of biogenic metal oxides nanoparticles. Inorganic and Nano-Metal Chemistry, 2018, 48, 441-448.	0.9	53
23	Discovery of novel oxindole derivatives as potent Î±-glucosidase inhibitors. Bioorganic and Medicinal Chemistry, 2014, 22, 3441-3448.	1.4	51
24	Hybrid benzothiazole analogs as antiurease agent: Synthesis and molecular docking studies. Bioorganic Chemistry, 2016, 66, 80-87.	2.0	51
25	Synthesis, in vitro alpha-glucosidase inhibitory potential of benzimidazole bearing bis-Schiff bases and their molecular docking study. Bioorganic Chemistry, 2020, 94, 103394.	2.0	51
26	Synthesis of new indazole based dual inhibitors of Î±-glucosidase and Î±-amylase enzymes, their in vitro, in silico and kinetics studies. Bioorganic Chemistry, 2020, 94, 103195.	2.0	51
27	Novel thiosemicarbazideâ€“oxadiazole hybrids as unprecedented inhibitors of yeast Î±-glucosidase and in silico binding analysis. RSC Advances, 2016, 6, 33733-33742.	1.7	49
28	2Ê¹-Aryl and 4Ê¹-arylidene substituted pyrazolones: As potential Î±-amylase inhibitors. European Journal of Medicinal Chemistry, 2018, 159, 47-58.	2.6	48
29	Evaluation of bisindole as potent Î²-glucuronidase inhibitors: Synthesis and in silico based studies. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 1825-1829.	1.0	47
30	Synthesis, Î±-glucosidase inhibitory, cytotoxicity and docking studies of 2-aryl-7-methylbenzimidazoles. Bioorganic Chemistry, 2016, 65, 100-109.	2.0	47
31	2-Aryl benzimidazoles: Synthesis, InÂvitro Î±-amylase inhibitory activity, and molecular docking study. European Journal of Medicinal Chemistry, 2018, 150, 248-260.	2.6	47
32	New Î±-Glucosidase inhibitors from the resins of Boswellia species with structureâ€“glucosidase activity and molecular docking studies. Bioorganic Chemistry, 2018, 79, 27-33.	2.0	46
33	Molecular modeling-based antioxidant arylidene barbiturates as urease inhibitors. Journal of Molecular Graphics and Modelling, 2011, 30, 153-156.	1.3	45
34	Synthesis of quinoline derivatives as diabetic II inhibitors and molecular docking studies. Bioorganic and Medicinal Chemistry, 2019, 27, 4081-4088.	1.4	45
35	Synthesis, in vitro urease inhibitory potential and molecular docking study of Benzimidazole analogues. Bioorganic Chemistry, 2019, 89, 103024.	2.0	45
36	Synthesis, in vitro biological activities and in silico study of dihydropyrimidines derivatives. Bioorganic and Medicinal Chemistry, 2015, 23, 6740-6748.	1.4	42

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37	Syntheses, in vitro Î±-amylase and Î±-glucosidase dual inhibitory activities of 4-amino-1,2,4-triazole derivatives their molecular docking and kinetic studies. Bioorganic and Medicinal Chemistry, 2020, 28, 115467.	1.4	42
38	Synthesis, in vitro evaluation and molecular docking studies of biscoumarin thiourea as a new inhibitor of Î±-glucosidases. Bioorganic Chemistry, 2015, 63, 36-44.	2.0	41
39	Synthesis, molecular docking studies of hybrid benzimidazole as Î± -glucosidase inhibitor. Bioorganic Chemistry, 2017, 70, 184-191.	2.0	40
40	Dihydropyrimidones: As novel class of Î²-glucuronidase inhibitors. Bioorganic and Medicinal Chemistry, 2016, 24, 3624-3635.	1.4	39
41	Chalcones and bis-chalcones: As potential Î±-amylase inhibitors; synthesis, in vitro screening, and molecular modelling studies. Bioorganic Chemistry, 2018, 79, 179-189.	2.0	39
42	In-vivo antinociceptive, anti-inflammatory and antipyretic activity of pistagremic acid isolated from Pistacia integerrima. Phytomedicine, 2014, 21, 1509-1515.	2.3	38
43	Selective glycosidase inhibitors: A patent review (2012â€“present). International Journal of Biological Macromolecules, 2018, 111, 82-91.	3.6	38
44	Flurbiprofen derivatives as novel Î±-amylase inhibitors: Biology-oriented drug synthesis (BIODS), in vitro, and in silico evaluation. Bioorganic Chemistry, 2018, 81, 157-167.	2.0	38
45	New triazinoindole bearing thiazole/oxazole analogues: Synthesis, Î±-amylase inhibitory potential and molecular docking study. Bioorganic Chemistry, 2019, 92, 103284.	2.0	38
46	The Landscape of Protein Tyrosine Phosphatase (Shp2) and Cancer. Current Pharmaceutical Design, 2019, 24, 3767-3777.	0.9	38
47	Synthesis, in vitro Î±-glucosidase inhibitory activity and molecular docking studies of new thiazole derivatives. Bioorganic Chemistry, 2016, 68, 245-258.	2.0	37
48	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
49	Gain-of-Function SHP2 E76Q Mutant Rescuing Autoinhibition Mechanism Associated with Juvenile Myelomonocytic Leukemia. Journal of Chemical Information and Modeling, 2019, 59, 3229-3239.	2.5	37
50	New Hybrid Scaffolds based on Hydrazinyl Thiazole Substituted Coumarin; As Novel Leads of Dual Potential; In Vitro Î±-Amylase Inhibitory and Antioxidant (DPPH and ABTS Radical Scavenging) Activities. Medicinal Chemistry, 2019, 15, 87-101.	0.7	37
51	Dihydropyrimidine based hydrazine dihydrochloride derivatives as potent urease inhibitors. Bioorganic Chemistry, 2016, 64, 85-96.	2.0	35
52	Synthesis, in vitro Î±-amylase inhibitory, and radicals (DPPH & ABTS) scavenging potentials of new N-sulfonohydrazide substituted indazoles. Bioorganic Chemistry, 2020, 94, 103410.	2.0	34
53	Synthesis, molecular docking study and in vitro thymidine phosphorylase inhibitory potential of oxadiazole derivatives. Bioorganic Chemistry, 2018, 78, 58-67.	2.0	33
54	Synthesis of new arylhydrazide bearing Schiff bases/thiazolidinone: Î±-Amylase, urease activities and their molecular docking studies. Bioorganic Chemistry, 2019, 91, 103112.	2.0	33

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55	Synthesis, in vitro urease inhibitory potential and molecular docking study of benzofuran-based-thiazoldinone analogues. Scientific Reports, 2020, 10, 10673.	1.6	33
56	Metabolic pathway analysis approach: Identification of novel therapeutic target against methicillin resistant Staphylococcus aureus. Gene, 2015, 556, 213-226.	1.0	31
57	Syntheses, in vitro evaluation and molecular docking studies of 5-bromo-2-aryl benzimidazoles as Î±-glucosidase inhibitors. Medicinal Chemistry Research, 2016, 25, 2058-2069.	1.1	31
58	Synthesis and molecular docking study of piperazine derivatives as potent urease inhibitors. Bioorganic Chemistry, 2018, 78, 411-417.	2.0	31
59	In-silico design of peptide inhibitors of K-Ras target in cancer disease. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5488-5499.	2.0	31
60	In Silico Identification and Evaluation of Leads for the Simultaneous Inhibition of Protease and Helicase Activities of HCV NS3/4A Protease Using Complex Based Pharmacophore Mapping and Virtual Screening. PLoS ONE, 2014, 9, e89109.	1.1	31
61	Synthesis, In vitro Î±-Glucosidase Inhibitory Potential and Molecular Docking Studies of 2-Amino-1,3,4-Oxadiazole Derivatives. Medicinal Chemistry, 2020, 16, 724-734.	0.7	31
62	Epitopes based drug design for dengue virus envelope protein: A computational approach. Computational Biology and Chemistry, 2017, 71, 152-160.	1.1	30
63	Norditerpenoid alkaloids of Delphinium denudatum as cholinesterase inhibitors. Bioorganic Chemistry, 2018, 78, 427-435.	2.0	29
64	Spectroscopic characterizations, structural peculiarities, molecular docking study and evaluation of biological potential of newly designed organotin(IV) carboxylates. Journal of Photochemistry and Photobiology B: Biology, 2019, 197, 111516.	1.7	29
65	Synthesis and screening of (E)-3-(2-benzylidenehydrazinyl)-5,6-diphenyl-1,2,4-triazine analogs as novel dual inhibitors of Î±-amylase and Î±-glucosidase. Bioorganic Chemistry, 2020, 101, 103979.	2.0	29
66	Targeting Dengue Virus NS-3 Helicase by Ligand based Pharmacophore Modeling and Structure based Virtual Screening. Frontiers in Chemistry, 2017, 5, 88.	1.8	28
67	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
68	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
69	Exploring the Pyrazinamide Drug Resistance Mechanism of Clinical Mutants T370P and W403G in Ribosomal Protein S1 of Mycobacterium tuberculosis. Journal of Chemical Information and Modeling, 2019, 59, 1584-1597.	2.5	26
70	Decoding allosteric communication pathways in protein lysine acetyltransferase. International Journal of Biological Macromolecules, 2020, 149, 70-80.	3.6	26
71	Thiadiazole derivatives as New Class of Î²-glucuronidase inhibitors. Bioorganic and Medicinal Chemistry, 2016, 24, 1909-1918.	1.4	25
72	Biology-oriented drug synthesis (BIODS): InÂvitro Î²-glucuronidase inhibitory and in silico studies on 2-(2-methyl-5-nitro-1H-imidazol-1-yl)ethyl aryl carboxylate derivatives. European Journal of Medicinal Chemistry, 2017, 125, 1289-1299.	2.6	25

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73	Metabolomic analysis of quorum sensing inhibitor hordenine on Pseudomonas aeruginosa. Applied Microbiology and Biotechnology, 2019, 103, 6271-6285.	1.7	25
74	Synthesis of novel quinoline-based thiadiazole, evaluation of their antileishmanial potential and molecular docking studies. Bioorganic Chemistry, 2019, 85, 109-116.	2.0	25
75	Synthesis of potent urease inhibitors based on disulfide scaffold and their molecular docking studies. Bioorganic and Medicinal Chemistry, 2015, 23, 7211-7218.	1.4	23
76	Atenolol thiourea hybrid as potent urease inhibitors: Design, biology-oriented drug synthesis, inhibitory activity screening, and molecular docking studies. Bioorganic Chemistry, 2020, 94, 103359.	2.0	23
77	Potent Î±-amylase inhibitors and radical (DPPH and ABTS) scavengers based on benzofuran-2-yl(phenyl)methanone derivatives: Syntheses, in vitro, kinetics, and in silico studies. Bioorganic Chemistry, 2020, 104, 104238.	2.0	23
78	Synthesis of indole derivatives as diabetics II inhibitors and enzymatic kinetics study of Î±-glucosidase and Î±-amylase along with their in-silico study. International Journal of Biological Macromolecules, 2021, 190, 301-318.	3.6	23
79	Underlying Anticancer Mechanisms and Synergistic Combinations of Phytochemicals with Cancer Chemotherapeutics: Potential Benefits and Risks. Journal of Food Quality, 2022, 2022, 1-15.	1.4	23
80	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
81	Mechanism of zinc ejection by disulfiram in nonstructural protein 5A. Physical Chemistry Chemical Physics, 2021, 23, 12204-12215.	1.3	22
82	Indole-3-acetamides: As Potential Antihyperglycemic and Antioxidant Agents; Synthesis, In Vitro Î±-Amylase Inhibitory Activity, Structureâ€“Activity Relationship, and In Silico Studies. ACS Omega, 2021, 6, 2264-2275.	1.6	22
83	In Silico Drug Designing for ala438 Deleted Ribosomal Protein S1 (RpsA) on the Basis of the Active Compound Zrl15. ACS Omega, 2022, 7, 397-408.	1.6	22
84	Molecular docking study of P4-Benzoxaborole-substituted ligands as inhibitors of HCV NS3/4A protease. Bioinformation, 2013, 9, 309-314.	0.2	21
85	Cytotoxicity, anti-angiogenic, anti-tumor and molecular docking studies on phytochemicals isolated from Polygonum hydropiper L.. BMC Complementary Medicine and Therapies, 2021, 21, 239.	1.2	21
86	Synthesis, SAR elucidations and molecular docking study of newly designed isatin based oxadiazole analogs as potent inhibitors of thymidine phosphorylase. Bioorganic Chemistry, 2018, 79, 323-333.	2.0	20
87	In silico identification of novel inhibitors against Plasmodium falciparum dihydroorate dehydrogenase. Journal of Molecular Graphics and Modelling, 2013, 40, 40-47.	1.3	19
88	Computational analysis of benzofuran-2-carboxlic acids as potent Pim-1 kinase inhibitors. Pharmaceutical Biology, 2014, 52, 1170-1178.	1.3	19
89	Genotyping of HCV RNA Reveals That 3a Is the Most Prevalent Genotype in Mardan, Pakistan. Advances in Virology, 2014, 2014, 1-5.	0.5	19
90	Urease inhibitory activity of ursane type sulfated saponins from the aerial parts of Zygophyllum fabago Linn. Phytomedicine, 2014, 21, 379-382.	2.3	19

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91	1-[(4â€²-Chlorophenyl) carbonyl-4-(aryl) thiosemicarbazide derivatives as potent urease inhibitors: Synthesis, in vitro and in silico studies. Bioorganic Chemistry, 2018, 79, 363-371.	2.0	19
92	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
93	Schiff bases of tryptamine as potent inhibitors of nucleoside triphosphate diphosphohydrolases (NTPDases): Structure-activity relationship. Bioorganic Chemistry, 2019, 82, 253-266.	2.0	19
94	Biology-oriented drug synthesis (BIODS), in vitro urease inhibitory activity, and in silico study of S-naproxen derivatives. Bioorganic Chemistry, 2019, 83, 29-46.	2.0	19
95	A New Urease Inhibitor from Viola betonicifolia. Molecules, 2014, 19, 16770-16778.	1.7	18
96	Allosteric mechanism of cyclopropylindolobenzazepine inhibitors for HCV NS5B RdRp via dynamic correlation network analysis. Molecular BioSystems, 2016, 12, 3280-3293.	2.9	18
97	Symmetrical and unsymmetrical substituted 2,5-diarylidene cyclohexanones as anti-parasitic compounds. European Journal of Medicinal Chemistry, 2018, 155, 596-608.	2.6	17
98	Synthesis, in vitro $$alpha $$ Î± -glucosidase inhibitory activity, and in silico study of (E)-thiosemicarbazones and (E)-2-(2-(arylmethylene)hydrazinyl)-4-arylthiazole derivatives. Molecular Diversity, 2018, 22, 841-861.	2.1	17
99	Subtractive proteomics and immunoinformatics approaches to explore Bartonella bacilliformis proteome (virulence factors) to design B and T cell multi-epitope subunit vaccine. Infection, Genetics and Evolution, 2020, 85, 104551.	1.0	17
100	Antibacterial, Antifungal, Antioxidant, and Docking Studies of Potential Dinaphthodiospyrols from Diospyros lotus Linn Roots. ACS Omega, 2021, 6, 5878-5885.	1.6	17
101	Synthesis and molecular docking study of piperazine derivatives as potent inhibitor of thymidine phosphorylase. Bioorganic Chemistry, 2018, 78, 324-331.	2.0	15
102	In-silico evaluations of the isolated phytosterols from polygonum hydropiper L against BACE1 and MAO drug targets. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10230-10238.	2.0	15
103	Whole exome analysis reveals a novel missense PNPLA1 variant that causes autosomal recessive congenital ichthyosis in a Pakistani family. Journal of Dermatological Science, 2016, 82, 46-48.	1.0	14
104	Synthesis, inÂvitro Î² -glucuronidase inhibitory potential and molecular docking studies of quinolines. European Journal of Medicinal Chemistry, 2017, 139, 849-864.	2.6	14
105	Natural compounds from plants controlling leishmanial growth via DNA damage and inhibiting trypanothione reductase and trypanothione synthetase: an in vitro and in silico approach. 3 Biotech, 2019, 9, 303.	1.1	14
106	In Silico, Cytotoxic and Antioxidant Potential of Novel Ester, 3-hydroxyoctyl -5-trans-docosenoate Isolated from Anchusa arvensis (L.) M.Bieb. Against HepG-2 Cancer Cells . Drug Design, Development and Therapy, 2019, Volume 13, 4195-4205.	2.0	14
107	Substituted Benzimidazole Analogues as Potential Î±-Amylase Inhibitors and Radical Scavengers. ACS Omega, 2021, 6, 22726-22739.	1.6	14
108	Molecular modeling and molecular dynamics simulation study of the human Rab9 and RhoBTB3 C-terminus complex. Bioinformation, 2014, 10, 757-763.	0.2	13

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109	Structural and spectral investigations of the recently synthesized chalcone (E)-3-mesityl-1-(naphthalen-2-yl) prop-2-en-1-one, a potential chemotherapeutic agent. Chemistry Central Journal, 2015, 9, 35.	2.6	13
110	Synthesis of oxadiazole-coupled-thiadiazole derivatives as a potent Î²-glucuronidase inhibitors and their molecular docking study. Bioorganic and Medicinal Chemistry, 2019, 27, 3145-3155.	1.4	13
111	Natural urease inhibitors from Aloe vera resin and Lycium shawii and their structural-activity relationship and molecular docking study. Bioorganic Chemistry, 2019, 88, 102955.	2.0	13
112	Hidden allosteric sites and De-Novo drug design. Expert Opinion on Drug Discovery, 2022, 17, 283-295.	2.5	13
113	New Diethyl Ammonium Salt of Thiobarbituric Acid Derivative: Synthesis, Molecular Structure Investigations and Docking Studies. Molecules, 2015, 20, 20642-20658.	1.7	12
114	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
115	In silico binding analysis and SAR elucidations of newly designed benzopyrazine analogs as potent inhibitors of thymidine phosphorylase. Bioorganic Chemistry, 2016, 68, 80-89.	2.0	12
116	Structure-Based Virtual Screening of Tumor Necrosis Factor-Î± Inhibitors by Cheminformatics Approaches and Bio-Molecular Simulation. Biomolecules, 2021, 11, 329.	1.8	12
117	New isolate from <scp>Salvinia molesta</scp> with antioxidant and urease inhibitory activity. Drug Development Research, 2021, 82, 1169-1181.	1.4	12
118	Synthesis, Molecular Modeling and Biological Evaluation of 5-arylidene-N,N-diethylthiobarbiturates as Potential Î±-glucosidase Inhibitors. Medicinal Chemistry, 2019, 15, 175-185.	0.7	12
119	New biologically dynamic hybrid pharmacophore triazinoindole-based-thiadiazole as potent Î±-glucosidase inhibitors: In vitro and in silico study. International Journal of Biological Macromolecules, 2022, 199, 77-85.	3.6	12
120	Biological properties of Hertia cheirifolia L. flower extracts and effect of the nopol on Î±-glucosidase. International Journal of Biological Macromolecules, 2017, 95, 757-761.	3.6	11
121	Synthesis, characterization, antioxidant, antileishmanial, anticancer, DNA and theoretical SARS-CoV-2 interaction studies of copper(II) carboxylate complexes. Journal of Molecular Structure, 2022, 1253, 132308.	1.8	11
122	Design, synthesis, in vitro evaluation, and docking studies on ibuprofen derived 1,3,4-oxadiazole derivatives as dual Î±-glucosidase and urease inhibitors. Medicinal Chemistry Research, 2022, 31, 316-336.	1.1	11
123	Synthesis, docking studies, and in silico ADMET predictions of some new derivatives of pyrimidine as potential KSP inhibitors. Medicinal Chemistry Research, 2015, 24, 304-315.	1.1	10
124	Synthesis of novel disulfide and sulfone hybrid scaffolds as potent Î²-glucuronidase inhibitor. Bioorganic Chemistry, 2016, 68, 15-22.	2.0	10
125	Predicting Multi-Interfacial Binding Mechanisms of NLRP3 and ASC Pyrin Domains in Inflammasome Activation. ACS Chemical Neuroscience, 2021, 12, 603-612.	1.7	10
126	Computational identification of potential drug targets against Mycobacterium leprae. Medicinal Chemistry Research, 2016, 25, 473-481.	1.1	9

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127	Synthesis, in vitro Î² -glucuronidase inhibitory activity and in silico studies of novel (E) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 7	2.0	9
128	Anti-Dengue, Cytotoxicity, Antifungal, and In Silico Study of the Newly Synthesized 3-O-Phospo-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="M1"><mml:mrow><mml:mtext mathvariant="bold">Î±</mml:mtext></mml:mrow></mml:math>-D-Glucopyranuronic Acid Compound. BioMed Research International, 2018, 2018, 1-5.	0.9	9
129	In Vivo Study on Analgesic, Muscle-Relaxant, Sedative Activity of Extracts of Hypochaeris radicata and In Silico Evaluation of Certain Compounds Present in This Species. BioMed Research International, 2018, 2018, 1-10.	0.9	9
130	1,1'-Carbonyldiimidazole (CDI) Mediated Facile Synthesis, Structural Characterization, Antimicrobial Activity, and in-silico Studies of Coumarin- 3-carboxamide Derivatives. Medicinal Chemistry, 2018, 14, 86-101.	0.7	9
131	Synthesis of new isoquinoline-base-oxadiazole derivatives as potent inhibitors of thymidine phosphorylase and molecular docking study. Scientific Reports, 2019, 9, 16015.	1.6	9
132	N-Aryl-3,4-dihydroisoquinoline Carbothioamide Analogues as Potential Urease Inhibitors. ACS Omega, 2021, 6, 15794-15803.	1.6	9
133	Synthesis,inÂvitrobiological screening and docking study of benzo[d]oxazolebisSchiff base derivatives as a potent anti-Alzheimer agent. Journal of Biomolecular Structure and Dynamics, 2023, 41, 1649-1664.	2.0	9
134	Synthesis, X-Ray Crystal Structures, Biological Evaluation, and Molecular Docking Studies of a Series of Barbiturate Derivatives. Journal of Chemistry, 2016, 2016, 1-11.	0.9	8
135	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
136	Synthesis, thymidine phosphorylase, angiogenic inhibition and molecular docking study of isoquinoline derivatives. Bioorganic Chemistry, 2019, 89, 102999.	2.0	8
137	Chalcones: As Potent Î±-amylase Enzyme Inhibitors; Synthesis, In Vitro, and In Silico Studies. Medicinal Chemistry, 2021, 17, 903-912.	0.7	8
138	Computational screening and analysis of deleterious nsSNPs in human p14ARF (CDKN2A) Tj ETQq0 0 0 rgBT /Overlock 10 Dynamics, 2023, 41, 3964-3975.	2.0	8
139	Binding site identification and role of permanent water molecule of PIM-3 kinase: A molecular dynamics study. Journal of Molecular Graphics and Modelling, 2015, 62, 276-282.	1.3	7
140	3,4-Dimethoxybenzohydrazide derivatives as antiulcer: Molecular modeling and density functional studies. Bioorganic Chemistry, 2017, 75, 235-241.	2.0	7
141	Dihydroquinazolin-4(1H)-one derivatives as novel and potential leads for diabetic management. Molecular Diversity, 2022, 26, 849-868.	2.1	7
142	Synthesis, in vitro antiurease, in vivo antinematodal activity of quinoline analogs and their in-silico study. Bioorganic Chemistry, 2021, 115, 105199.	2.0	7
143	In vitro Î±-Glucosidase Inhibition by Non-sugar based Triazoles of Dibenzoazepine, their Structure-Activity Relationship, and Molecular Docking. Medicinal Chemistry, 2017, 13, 698-704.	0.7	7
144	Heparin-Assisted Amyloidogenesis Uncovered through Molecular Dynamics Simulations. ACS Omega, 2022, 7, 15132-15144.	1.6	7

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145	Three-dimensional quantitative structureâ€“activity relationship (CoMSIA) analysis of bis-coumerine analogues as urease inhibitors. Medicinal Chemistry Research, 2013, 22, 498-504.	1.1	6
146	Theoretical and Experimental in vitro Antifungal and Antitumor Activities of Organotin(IV) Derivatives of 3-(4-nitrophenyl)-2-methylacrylic acid. Pharmaceutical Chemistry Journal, 2019, 53, 689-696.	0.3	6
147	The in silico identification of small molecules for protein-protein interaction inhibition in AKAP-Lbcâ€“RhoA signaling complex. Computational Biology and Chemistry, 2017, 67, 84-91.	1.1	5
148	Modeling Novel Putative Drugs and Vaccine Candidates against Tick-Borne Pathogens: A Subtractive Proteomics Approach. Veterinary Sciences, 2020, 7, 129.	0.6	5
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