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	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
2	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
3	Dihydroquinazolin-4(1H)-one derivatives as novel and potential leads for diabetic management. Molecular Diversity, 2022, 26, 849-868.	2.1	7
4	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
5	Prospect of Anterior Gradient 2 homodimer inhibition via repurposing FDA-approved drugs using structure-based virtual screening. Molecular Diversity, 2022, 26, 1399-1409.	2.1	1
6	An effort to find new Î±-amylase inhibitors as potent antidiabetics compounds based on indole-based-thiadiazole analogs. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13103-13114.	2.0	4
7	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
8	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
9	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
10	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
11	Hidden allosteric sites and De-Novo drug design. Expert Opinion on Drug Discovery, 2022, 17, 283-295.	2.5	13
12	Heparin-Assisted Amyloidogenesis Uncovered through Molecular Dynamics Simulations. ACS Omega, 2022, 7, 15132-15144.	1.6	7
13	Strategies for Targeting KRAS: A Challenging Drug Target. Current Pharmaceutical Design, 2022, 28, 1897-1901.	0.9	4
14	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
15	Toward the Noninvasive Diagnosis of Alzheimerâ€™s Disease: Molecular Basis for the Specificity of Curcumin for Fibrillar Amyloid-Î². ACS Omega, 2022, 7, 22032-22038.	1.6	3
16	Urease and Î±-Chymotrypsin Inhibitory Activities and Molecular Docking Studies of Alkaloids Isolated from Medicinal Plant Isatis minima Bunge. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-10.	0.5	1
17	Synthesis, urease inhibition screening and molecular docking studies of piperonal based imine derivatives. Medicinal Chemistry Research, 2021, 30, 226-235.	1.1	5
18	Mechanism of zinc ejection by disulfiram in nonstructural protein 5A. Physical Chemistry Chemical Physics, 2021, 23, 12204-12215.	1.3	22

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19	Structure-Based Virtual Screening of Tumor Necrosis Factor-Î± Inhibitors by Cheminformatics Approaches and Bio-Molecular Simulation. Biomolecules, 2021, 11, 329.	1.8	12
20	Antibacterial, Antifungal, Antioxidant, and Docking Studies of Potential Dinaphthodiospyrols from Diospyros lotus Linn Roots. ACS Omega, 2021, 6, 5878-5885.	1.6	17
21	Computational Insight into the Binding Mechanism of Pyrazinoic Acid to RpsA Protein. Current Chinese Science, 2021, 1, 207-215.	0.2	2
22	New isolate from <scp>Salvinia molesta</scp> with antioxidant and urease inhibitory activity. Drug Development Research, 2021, 82, 1169-1181.	1.4	12
23	N-Aryl-3,4-dihydroisoquinoline Carbothioamide Analogues as Potential Urease Inhibitors. ACS Omega, 2021, 6, 15794-15803.	1.6	9
24	Substituted Benzimidazole Analogues as Potential Î±-Amylase Inhibitors and Radical Scavengers. ACS Omega, 2021, 6, 22726-22739.	1.6	14
25	Chalcones: As Potent Î±-amylase Enzyme Inhibitors; Synthesis, In Vitro, and In Silico Studies. Medicinal Chemistry, 2021, 17, 903-912.	0.7	8
26	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
27	2â€Mercapto Benzoxazole Derivatives as Novel Leads: Urease Inhibition, In Vitro and In Silico Studies. ChemistrySelect, 2021, 6, 8490-8498.	0.7	2
28	Synthesis, in vitro antiurease, in vivo antinematodal activity of quinoline analogs and their in-silico study. Bioorganic Chemistry, 2021, 115, 105199.	2.0	7
29	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
30	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
31	Predicting Multi-Interfacial Binding Mechanisms of NLRP3 and ASC Pyrin Domains in Inflammasome Activation. ACS Chemical Neuroscience, 2021, 12, 603-612.	1.7	10
32	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
33	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
34	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
35	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
36	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

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37	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
38	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
39	Synthesis, in vitro urease inhibitory potential and molecular docking study of benzofuran-based-thiazoldinone analogues. Scientific Reports, 2020, 10, 10673.	1.6	33
40	Modeling Novel Putative Drugs and Vaccine Candidates against Tick-Borne Pathogens: A Subtractive Proteomics Approach. Veterinary Sciences, 2020, 7, 129.	0.6	5
41	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
42	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
43	In Silico Modeling of Crimean Congo Hemorrhagic Fever Virus Glycoprotein-N and Screening of Anti Viral Hits by Virtual Screening. International Journal of Peptide Research and Therapeutics, 2020, 26, 2675-2688.	0.9	3
44	Functional annotation of regulatory single nucleotide polymorphisms associated with schizophrenia. Schizophrenia Research, 2020, 218, 326-328.	1.1	4
45	Decoding allosteric communication pathways in protein lysine acetyltransferase. International Journal of Biological Macromolecules, 2020, 149, 70-80.	3.6	26
46	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
47	Cytotoxicity of Anchusa arvensis Against HepG-2 Cell Lines: Mechanistic and Computational Approaches. Current Topics in Medicinal Chemistry, 2020, 19, 2805-2813.	1.0	5
48	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
49	Binuclear copper(II) complexes: Synthesis, structural characterization, DNA binding and in silico studies. Journal of the Serbian Chemical Society, 2020, 85, 751-764.	0.4	5
50	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
51	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
52	Synthesis of quinoline derivatives as diabetic II inhibitors and molecular docking studies. Bioorganic and Medicinal Chemistry, 2019, 27, 4081-4088.	1.4	45
53	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
54	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

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55	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
56	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
57	New triazinoindole bearing thiazole/oxazole analogues: Synthesis, Î±-amylase inhibitory potential and molecular docking study. Bioorganic Chemistry, 2019, 92, 103284.	2.0	38
58	Synthesis, thymidine phosphorylase, angiogenic inhibition and molecular docking study of isoquinoline derivatives. Bioorganic Chemistry, 2019, 89, 102999.	2.0	8
59	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
60	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
61	Synthesis, in vitro urease inhibitory potential and molecular docking study of Benzimidazole analogues. Bioorganic Chemistry, 2019, 89, 103024.	2.0	45
62	Metabolomic analysis of quorum sensing inhibitor hordenine on Pseudomonas aeruginosa. Applied Microbiology and Biotechnology, 2019, 103, 6271-6285.	1.7	25
63	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
64	Diorganotin(IV) carboxylates of 3-methylphenyl ethanoic acid: Synthesis, crystal structure, antibacterial, anticancer and molecular docking studies. Phosphorus, Sulfur and Silicon and the Related Elements, 2019, 194, 1067-1073.	0.8	3
65	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
66	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
67	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
68	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
69	The Landscape of Protein Tyrosine Phosphatase (Shp2) and Cancer. Current Pharmaceutical Design, 2019, 24, 3767-3777.	0.9	38
70	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
71	Synthesis of benzothiazole derivatives as a potent Î±-glucosidase inhibitor. Bioorganic Chemistry, 2019, 85, 33-48.	2.0	54
72	Synthesis of novel quinoline-based thiadiazole, evaluation of their antileishmanial potential and molecular docking studies. Bioorganic Chemistry, 2019, 85, 109-116.	2.0	25

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73	Schiff bases of tryptamine as potent inhibitors of nucleoside triphosphate diphosphohydrolases (NTPDases): Structure-activity relationship. Bioorganic Chemistry, 2019, 82, 253-266.	2.0	19
74	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
75	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
76	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
77	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
78	Synthesis, molecular docking study and in vitro thymidine phosphorylase inhibitory potential of oxadiazole derivatives. Bioorganic Chemistry, 2018, 78, 58-67.	2.0	33
79	Norditerpenoid alkaloids of Delphinium denudatum as cholinesterase inhibitors. Bioorganic Chemistry, 2018, 78, 427-435.	2.0	29
80	Synthesis and molecular docking study of piperazine derivatives as potent urease inhibitors. Bioorganic Chemistry, 2018, 78, 411-417.	2.0	31
81	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
82	Selective glycosidase inhibitors: A patent review (2012â€“present). International Journal of Biological Macromolecules, 2018, 111, 82-91.	3.6	38
83	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
84	Pathogens constancy, harbinger of nosocomial infection cum identification of resistant genes and drug designing. Computational Biology and Chemistry, 2018, 74, 347-359.	1.1	1
85	Synthesis and molecular docking study of piperazine derivatives as potent inhibitor of thymidine phosphorylase. Bioorganic Chemistry, 2018, 78, 324-331.	2.0	15
86	Synthesis, in vitro Î±-glucosidase inhibitory potential and molecular docking study of thiadiazole analogs. Bioorganic Chemistry, 2018, 78, 201-209.	2.0	65
87	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
88	Oxindole based oxadiazole hybrid analogs: Novel Î± -glucosidase inhibitors. Bioorganic Chemistry, 2018, 76, 273-280.	2.0	53
89	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
90	2Ê¹-Aryl and 4Ê¹-arylidene substituted pyrazolones: As potential Î±-amylase inhibitors. European Journal of Medicinal Chemistry, 2018, 159, 47-58.	2.6	48

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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	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
93	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
94	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
95	Anti-proliferative potential of cyclotetrapeptides from Bacillus velezensis RA5401 and their molecular docking on G-Protein-Coupled Receptors. Microbial Pathogenesis, 2018, 123, 419-425.	1.3	3
96	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
97	Antimicrobial efficiency of diorganotin(IV) bis-[3-(4-chlorophenyl)-2-methylacrylate]. Journal of Coordination Chemistry, 2018, 71, 3315-3329.	0.8	1
98	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
99	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
100	Symmetrical and unsymmetrical substituted 2,5-diarylidene cyclohexanones as anti-parasitic compounds. European Journal of Medicinal Chemistry, 2018, 155, 596-608.	2.6	17
101	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
102	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
103	2-Indolinone Derivatives as Potent Urease Inhibitors. Letters in Drug Design and Discovery, 2018, 15, 814-821.	0.4	1
104	Synthesis, in vitro Î² -glucuronidase inhibitory activity and in silico studies of novel (E) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 222 Td ()-4-	2.0	9
105	Antioxidant and anticholinesterase potential of diterpenoid alkaloids from Aconitum heterophyllum. Bioorganic and Medicinal Chemistry, 2017, 25, 3368-3376.	1.4	55
106	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
107	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
108	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

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109	Synthesis, molecular docking studies of hybrid benzimidazole as Î± -glucosidase inhibitor. Bioorganic Chemistry, 2017, 70, 184-191.	2.0	40
110	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
111	3,4-Dimethoxybenzohydrazide derivatives as antiulcer: Molecular modeling and density functional studies. Bioorganic Chemistry, 2017, 75, 235-241.	2.0	7
112	Epitopes based drug design for dengue virus envelope protein: A computational approach. Computational Biology and Chemistry, 2017, 71, 152-160.	1.1	30
113	Synthesis, inÂvitro Î² -glucuronidase inhibitory potential and molecular docking studies of quinolines. European Journal of Medicinal Chemistry, 2017, 139, 849-864.	2.6	14
114	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
115	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
116	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
117	Anti-Alzheimerâ€™s Studies on Î²-Sitosterol Isolated from Polygonum hydropiper L.. Frontiers in Pharmacology, 2017, 8, 697.	1.6	159
118	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
119	New Hybrid Hydrazinyl Thiazole Substituted Chromones: As Potential Î±-Amylase Inhibitors and Radical (DPPH & ABTS) Scavengers. Scientific Reports, 2017, 7, 16980.	1.6	70
120	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
121	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
122	Antimicrobial Activity of Some Novel Armed Thiophene Derivatives and Petra/Osiris/Molinspiration (POM) Analyses. Molecules, 2016, 21, 222.	1.7	86
123	Synthesis of novel disulfide and sulfone hybrid scaffolds as potent Î²-glucuronidase inhibitor. Bioorganic Chemistry, 2016, 68, 15-22.	2.0	10
124	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
125	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
126	Synthesis, Î²-glucuronidase inhibition and molecular docking studies of hybrid bisindole-thiosemicarbazides analogs. Bioorganic Chemistry, 2016, 68, 56-63.	2.0	66

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127	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
128	Allosteric mechanism of cyclopropylindolobenzazepine inhibitors for HCV NS5B RdRp via dynamic correlation network analysis. Molecular BioSystems, 2016, 12, 3280-3293.	2.9	18
129	Synthesis, in vitro Î±-glucosidase inhibitory activity and molecular docking studies of new thiazole derivatives. Bioorganic Chemistry, 2016, 68, 245-258.	2.0	37
130	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
131	Synthesis, Enzyme Inhibition, and Molecular Docking Studies of Hydrazones from Dichlorophenylacetic Acids. Journal of the Chinese Chemical Society, 2016, 63, 1015-1021.	0.8	2
132	Dihydropyrimidones: As novel class of Î²-glucuronidase inhibitors. Bioorganic and Medicinal Chemistry, 2016, 24, 3624-3635.	1.4	39
133	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
134	Computational identification of potential drug targets against Mycobacterium leprae. Medicinal Chemistry Research, 2016, 25, 473-481.	1.1	9
135	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
136	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
137	Hybrid benzothiazole analogs as antiurease agent: Synthesis and molecular docking studies. Bioorganic Chemistry, 2016, 66, 80-87.	2.0	51
138	Synthesis, Î±-glucosidase inhibitory, cytotoxicity and docking studies of 2-aryl-7-methylbenzimidazoles. Bioorganic Chemistry, 2016, 65, 100-109.	2.0	47
139	Thiadiazole derivatives as New Class of Î²-glucuronidase inhibitors. Bioorganic and Medicinal Chemistry, 2016, 24, 1909-1918.	1.4	25
140	Dihydropyrimidine based hydrazine dihydrochloride derivatives as potent urease inhibitors. Bioorganic Chemistry, 2016, 64, 85-96.	2.0	35
141	New Diethyl Ammonium Salt of Thiobarbituric Acid Derivative: Synthesis, Molecular Structure Investigations and Docking Studies. Molecules, 2015, 20, 20642-20658.	1.7	12
142	Novel quinoline derivatives as potent in vitro Î±-glucosidase inhibitors: in silico studies and SAR predictions. MedChemComm, 2015, 6, 1826-1836.	3.5	58
143	Metabolic pathway analysis approach: Identification of novel therapeutic target against methicillin resistant Staphylococcus aureus. Gene, 2015, 556, 213-226.	1.0	31
144	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

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145	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
146	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
147	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
148	Synthesis of 4-thiazolidinone analogs as potent in vitro anti-urease agents. Bioorganic Chemistry, 2015, 63, 123-131.	2.0	85
149	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
150	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
151	Synthesis, in vitro biological activities and in silico study of dihydropyrimidines derivatives. Bioorganic and Medicinal Chemistry, 2015, 23, 6740-6748.	1.4	42
152	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
153	Triazinoindole analogs as potent inhibitors of Î±-glucosidase: Synthesis, biological evaluation and molecular docking studies. Bioorganic Chemistry, 2015, 58, 81-87.	2.0	126
154	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
155	Molecular modeling and molecular dynamics simulation study of the human Rab9 and RhoBTB3 C-terminus complex. Bioinformation, 2014, 10, 757-763.	0.2	13
156	A New Urease Inhibitor from Viola betonicifolia. Molecules, 2014, 19, 16770-16778.	1.7	18
157	Computational analysis of benzofuran-2-carboxlic acids as potent Pim-1 kinase inhibitors. Pharmaceutical Biology, 2014, 52, 1170-1178.	1.3	19
158	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
159	Discovery of novel oxindole derivatives as potent Î±-glucosidase inhibitors. Bioorganic and Medicinal Chemistry, 2014, 22, 3441-3448.	1.4	51
160	Urease inhibitory activity of ursane type sulfated saponins from the aerial parts of Zygophyllum fabago Linn. Phytomedicine, 2014, 21, 379-382.	2.3	19
161	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
162	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

#	Article	IF	Citations
163	In-vivo antinociceptive, anti-inflammatory and antipyretic activity of pistagremic acid isolated from Pistacia integerrima. Phytomedicine, 2014, 21, 1509-1515.	2.3	38
164	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
165	Design of New and Potent Diethyl Thiobarbiturates as Urease Inhibitors: A Computational Approach. Bioinformation, 2014, 10, 299-307.	0.2	0
166	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
167	In silico identification of novel inhibitors against Plasmodium falciparum dihydroorate dehydrogenase. Journal of Molecular Graphics and Modelling, 2013, 40, 40-47.	1.3	19
168	Molecular docking study of P4-Benzoxaborole-substituted ligands as inhibitors of HCV NS3/4A protease. Bioinformation, 2013, 9, 309-314.	0.2	21
169	Molecular modeling-based antioxidant arylidene barbiturates as urease inhibitors. Journal of Molecular Graphics and Modelling, 2011, 30, 153-156.	1.3	45