Zaheer Ul-Haq

List of Publications by Year
in descending order

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189	3,708	147566	205818
papers	citations	31 h-index	48 g-index

196	196	196	5032
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Synthesis, antioxidant activities and urease inhibition of some new 1,2,4-triazole and 1,3,4-thiadiazole derivatives. European Journal of Medicinal Chemistry, 2010, 45, 5200-5207.	2.6	265
2	Identification of chymotrypsin-like protease inhibitors of SARS-CoV-2 via integrated computational approach. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2607-2616.	2.0	227
3	Withanolides, a new class of natural cholinesterase inhibitors with calcium antagonistic properties. Biochemical and Biophysical Research Communications, 2005, 334, 276-287.	1.0	92
4	Synthesis of novel inhibitors of Î²-glucuronidase based on benzothiazole skeleton and study of their binding affinity by molecular docking. Bioorganic and Medicinal Chemistry, 2011, 19, 4286-4294.	1.4	91
5	Juliflorine: A potent natural peripheral anionic-site-binding inhibitor of acetylcholinesterase with calcium-channel blocking potential, a leading candidate for Alzheimerâ€™s disease therapy. Biochemical and Biophysical Research Communications, 2005, 332, 1171-1179.	1.0	83
6	Identification of Novel Urease Inhibitors by High-Throughput Virtual and in Vitro Screening. ACS Medicinal Chemistry Letters, 2010, 1, 145-149.	1.3	71
7	Interleukin-4 receptor signaling and its binding mechanism: A therapeutic insight from inhibitors tool box. Cytokine and Growth Factor Reviews, 2016, 32, 3-15.	3.2	64
8	BRAF gene: From human cancers to developmental syndromes. Saudi Journal of Biological Sciences, 2015, 22, 359-373.	1.8	61
9	Presence of Antispasmodic, Antidiarrheal, Antisecretory, Calcium Antagonist and Acetylcholinesterase Inhibitory Steroidal Alkaloids inSarcococca saligna. Planta Medica, 2005, 71, 120-125.	0.7	59
10	Biological and molecular docking studies on coagulin-H: Human IL-2 novel natural inhibitor. Molecular Immunology, 2006, 43, 1855-1863.	1.0	56
11	Kinetics and structureâ€“activity relationship studies on pregnane-type steroidal alkaloids that inhibit cholinesterases. Bioorganic and Medicinal Chemistry, 2004, 12, 1995-2003.	1.4	47
12	Cholinesterase inhibitory and spasmolytic potential of steroidal alkaloids. Journal of Steroid Biochemistry and Molecular Biology, 2004, 92, 477-484.	1.2	45
13	Molecular modeling-based antioxidant arylidene barbiturates as urease inhibitors. Journal of Molecular Graphics and Modelling, 2011, 30, 153-156.	1.3	45
14	Catalytic asymmetric synthesis of indole derivatives as novel Î±-glucosidase inhibitors in vitro. Bioorganic Chemistry, 2018, 79, 350-354.	2.0	44
15	Î±-Glucosidase inhibitory effect of rhinacanthins-rich extract from Rhinacanthus nasutus leaf and synergistic effect in combination with acarbose. Journal of Functional Foods, 2017, 36, 325-331.	1.6	43
16	Pregnane-Type Steroidal Alkaloids ofSarcococca saligna: a New Class of Cholinesterase Inhibitors. Helvetica Chimica Acta, 2002, 85, 678-688.	1.0	42
17	Molecular Docking Studies of Natural Cholinesterase-Inhibiting Steroidal Alkaloids fromSarcococcasaligna. Journal of Medicinal Chemistry, 2003, 46, 5087-5090.	2.9	42
18	Identification of potent urease inhibitors via ligand- and structure-based virtual screening and in vitro assays. Journal of Molecular Graphics and Modelling, 2010, 28, 792-798.	1.3	42

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19	Synthesis of pyrimidine-2,4,6-trione derivatives: Anti-oxidant, anti-cancer, Î±-glucosidase, Î²-glucuronidase inhibition and their molecular docking studies. Bioorganic Chemistry, 2016, 68, 72-79.	2.0	42
20	5-Acetyl-6-methyl-4-aryl-3,4-dihydropyrimidin-2(1 H)-ones: As potent urease inhibitors; synthesis, in vitro screening, and molecular modeling study. Bioorganic Chemistry, 2018, 76, 37-52.	2.0	41
21	Indole acrylonitriles as potential anti-hyperglycemic agents: Synthesis, Î±-glucosidase inhibitory activity and molecular docking studies. Bioorganic and Medicinal Chemistry, 2020, 28, 115605.	1.4	41
22	New Cholinesterase-Inhibiting Steroidal Alkaloids fromSarcococca saligna. Helvetica Chimica Acta, 2004, 87, 439-448.	1.0	40
23	Synthesis and biological activity of oxadiazole and triazolothiadiazole derivatives as tyrosinase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 3755-3759.	1.0	40
24	Identification of potential TNF-Î± inhibitors: from in silico to in vitro studies. Scientific Reports, 2020, 10, 20974.	1.6	39
25	Synthesis of azachalcones, their Î±-amylase, Î±-glucosidase inhibitory activities, kinetics, and molecular docking studies. Bioorganic Chemistry, 2021, 106, 104489.	2.0	39
26	New pregnane-type steroidal alkaloids from Sarcococca saligna and their cholinesterase inhibitory activity. Steroids, 2004, 69, 735-741.	0.8	37
27	Receptor-Based Modeling and 3D-QSAR for a Quantitative Production of the Butyrylcholinesterase Inhibitors Based on Genetic Algorithm. Journal of Chemical Information and Modeling, 2008, 48, 1092-1103.	2.5	37
28	Eriodictyol stimulates insulin secretion through cAMP/PKA signaling pathway in mice islets. European Journal of Pharmacology, 2018, 820, 245-255.	1.7	37
29	3D-QSAR CoMFA studies on bis-coumarine analogues as urease inhibitors: A strategic design in anti-urease agents. Bioorganic and Medicinal Chemistry, 2008, 16, 3456-3461.	1.4	36
30	Design and synthesis of chalcone derivatives as potent tyrosinase inhibitors and their structural activity relationship. Journal of Molecular Structure, 2015, 1085, 97-103.	1.8	35
31	Development of sulfonamide-based Schiff bases targeting urease inhibition: Synthesis, characterization, inhibitory activity assessment, molecular docking and ADME studies. Bioorganic Chemistry, 2020, 102, 104057.	2.0	35
32	Structure-based design, synthesis and biological evaluation of Î²-glucuronidase inhibitors. Journal of Computer-Aided Molecular Design, 2014, 28, 577-585.	1.3	33
33	3D-QSAR Studies on natural acetylcholinesterase inhibitors of Sarcococca saligna by comparative molecular field analysis (CoMFA). Bioorganic and Medicinal Chemistry Letters, 2003, 13, 4375-4380.	1.0	31
34	First ComprehensiveIn SilicoAnalysis of the Functional and Structural Consequences of SNPs in HumanGalNAc-T1Gene. Computational and Mathematical Methods in Medicine, 2014, 2014, 1-15.	0.7	31
35	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
36	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

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37	In silico modeling of the specific inhibitory potential of thiophene-2,3-dihydro-1,5-benzothiazepine against BChE in the formation of Î²-amyloid plaques associated with Alzheimer's disease. Theoretical Biology and Medical Modelling, 2010, 7, 22.	2.1	29
38	Structure based virtual screening-driven identification of monastrol as a potent urease inhibitor. Journal of Molecular Graphics and Modelling, 2013, 43, 47-57.	1.3	29
39	The immunomodulation potential of the synthetic derivatives of benzothiazoles: Implications in immune system disorders through in vitro and in silico studies. Bioorganic Chemistry, 2016, 64, 21-28.	2.0	28
40	Synthesis, and In Vitro and In Silico Î±-Glucosidase Inhibitory Studies of 5-Chloro-2-Aryl Benzo[d]thiazoles. Bioorganic Chemistry, 2018, 78, 269-279.	2.0	28
41	Synthesis, antimicrobial activity, pharmacophore modeling and molecular docking studies of new pyrazole-dimedone hybrid architectures. Chemistry Central Journal, 2018, 12, 29.	2.6	28
42	Coumarin derivatives as acetyl- and butyrylcholinestrase inhibitors: An inÂvitro, molecular docking, and molecular dynamics simulations study. Heliyon, 2019, 5, e01552.	1.4	28
43	In Silico and In Vitro Immunomodulatory Studies on Compounds of Lindelofia stylosa. Chemical Biology and Drug Design, 2012, 79, 290-299.	1.5	27
44	Benchmarking docking and scoring protocol for the identification of potential acetylcholinesterase inhibitors. Journal of Molecular Graphics and Modelling, 2010, 28, 870-882.	1.3	25
45	Synthesis of thiobarbituric acid derivatives: In vitro Î± -glucosidase inhibition and molecular docking studies. Bioorganic Chemistry, 2017, 75, 99-105.	2.0	25
46	Anti-hyperglycemic and anti-hyperlipidemic effects of rhinacanthins-rich extract from Rhinacanthus nasutus leaves in nicotinamide-streptozotocin induced diabetic rats. Biomedicine and Pharmacotherapy, 2019, 113, 108702.	2.5	25
47	Natural flavonoid Î±-glucosidase inhibitors from Retama raetam: Enzyme inhibition and molecular docking reveal important interactions with the enzyme active site. Bioorganic Chemistry, 2019, 87, 736-742.	2.0	25
48	Immunosuppressive Activity of Buxidin and Eâ€Buxenone from Buxus hyrcana. Chemical Biology and Drug Design, 2010, 75, 310-317.	1.5	24
49	Bioisosteric approach in designing new monastrol derivatives: An investigation on their ADMET prediction using in silico derived parameters. Journal of Molecular Graphics and Modelling, 2013, 45, 202-210.	1.3	24
50	Synthesis and dynamics studies of barbituric acid derivatives as urease inhibitors. Chemistry Central Journal, 2015, 9, 63.	2.6	23
51	Design, Synthesis and Docking Studies of Flavokawain B Type Chalcones and Their Cytotoxic Effects on MCF-7 and MDA-MB-231 Cell Lines. Molecules, 2018, 23, 616.	1.7	23
52	Molecular and structural determinants of adamantyl susceptibility to HLA-DRs allelic variants: an in silico approach to understand the mechanism of MLEs. Journal of Computer-Aided Molecular Design, 2011, 25, 81-101.	1.3	22
53	Molecular docking studies of potent inhibitors of tyrosinase and Î±-glucosidase. Medicinal Chemistry Research, 2012, 21, 1677-1683.	1.1	22
54	Purification and Characterization of a Nonspecific Lipid Transfer Protein 1 (nsLTP1) from Ajwain (Trachyspermum ammi) Seeds. Scientific Reports, 2019, 9, 4148.	1.6	21

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55	Successful computer guided planned synthesis of (4R)-thiazolidine carboxylic acid and its 2-substituted analogues as urease inhibitors. Molecular Diversity, 2006, 10, 223-231.	2.1	20
56	Synthesis, Bioactivity, Molecular Docking and POM Analyses of Novel Substituted Thieno[2,3-b]thiophenes and Related Congeners. Molecules, 2015, 20, 1824-1841.	1.7	20
57	Synthetic flavonoids as potential antiviral agents against SARS-CoV-2 main protease. Journal of Biomolecular Structure and Dynamics, 2022, 40, 3777-3788.	2.0	20
58	Family 18 chitolectins: Comparison of MGP40 and HUMGP39. Biochemical and Biophysical Research Communications, 2007, 359, 221-226.	1.0	19
59	In silico identification of novel inhibitors against Plasmodium falciparum dihydroorate dehydrogenase. Journal of Molecular Graphics and Modelling, 2013, 40, 40-47.	1.3	19
60	Synthesis, Anti-microbial and Molecular Docking Studies of Quinazolin-4(3H)-one Derivatives. Molecules, 2014, 19, 8725-8739.	1.7	19
61	Structure based 3D-QSAR studies of Interleukin-2 inhibitors: Comparing the quality and predictivity of 3D-QSAR models obtained from different alignment methods and charge calculations. Chemico-Biological Interactions, 2015, 238, 9-24.	1.7	19
62	Superoxide scavenging and antiglycation activity of rhinacanthins-rich extract obtained from the leaves of Rhinacanthus nasutus. Pharmacognosy Magazine, 2017, 13, 652.	0.3	19
63	CoMFA and CoMSIA 3D-QSAR analysis on hydroxamic acid derivatives as urease inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2009, 24, 272-278.	2.5	18
64	Molecular dynamics simulation of mammalian 15S-lipoxygenase with AMBER force field. European Biophysics Journal, 2011, 40, 715-726.	1.2	18
65	Identification of novel Interleukin-2 inhibitors through computational approaches. Molecular Diversity, 2013, 17, 345-355.	2.1	18
66	Synthesis, crystal structure, evaluation of urease inhibition potential and the docking studies of cobalt(III) complex based on barbituric acid Schiff base ligand. Inorganica Chimica Acta, 2020, 503, 119405.	1.2	18
67	Ligandâ€based 3Dâ€QSAR Studies of Physostigmine Analogues as Acetylcholinesterase Inhibitors. Chemical Biology and Drug Design, 2009, 74, 571-581.	1.5	17
68	Human serum albumin-specific recognition of the natural herbal extract of Stryphnodendron polyphyllum through STD NMR, hyphenations and docking simulation studies. RSC Advances, 2015, 5, 23431-23442.	1.7	17
69	Biomolecular interactions of amphotericin B nanomicelles with serum albumins: A combined biophysical and molecular docking approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 205, 442-456.	2.0	17
70	Synthesis and characterisation of thiobarbituric acid enamine derivatives, and evaluation of their Î±-glucosidase inhibitory and anti-glycation activity. Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 692-701.	2.5	17
71	Biology-oriented drug synthesis (BIODS), in vitro urease inhibitory activity, and in silico studies on ibuprofen derivatives. Molecular Diversity, 2021, 25, 143-157.	2.1	17
72	2-Mercapto Benzothiazole Derivatives: As Potential Leads for the Diabetic Management. Medicinal Chemistry, 2020, 16, 826-840.	0.7	17

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73	Combined Pharmacophore and 3Dâ€QSAR Study on A Series of Staphylococcus aureus Sortase A inhibitors. Chemical Biology and Drug Design, 2012, 80, 300-314.	1.5	16
74	Brine shrimp lethality assay â€˜an effective prescreenâ€™: Microwave-assisted synthesis, BSL toxicity and 3DQSAR studies-based designing, docking and antitumor evaluation of potent chalcones. Pharmaceutical Biology, 2013, 51, 1091-1103.	1.3	16
75	Evaluation of binding competition and group epitopes of acetylcholinesterase inhibitors by STD NMR, Tr-NOESY, DOSY and molecular docking: an old approach but new findings. MedChemComm, 2015, 6, 1882-1890.	3.5	16
76	Bioactivity, Safety, and Efficacy of Amphotericin B Nanomicellar Aerosols Using Sodium Deoxycholate Sulfate as the Lipid Carrier. AAPS PharmSciTech, 2018, 19, 2077-2086.	1.5	16
77	Synthesis of Oxindole Analogues, Biological Activity, and In Silico Studies. ChemistrySelect, 2019, 4, 10510-10516.	0.7	16
78	Synthesis of a New Class of Spirooxindoleâ€“Benzo[b]Thiophene-Based Molecules as Acetylcholinesterase Inhibitors. Molecules, 2020, 25, 4671.	1.7	16
79	An in-silico evaluation of COVID-19 main protease with clinically approved drugs. Journal of Molecular Graphics and Modelling, 2020, 101, 107758.	1.3	16
80	Synthesis, biological evaluation, and molecular docking studies of benzyl, alkyl and glycosyl [2-(arylamino)-4,4-dimethyl-6-oxo-cyclohex-1-ene]carbodithioates, as potential immunomodulatory and immunosuppressive agents. Bioorganic and Medicinal Chemistry, 2012, 20, 3000-3008.	1.4	15
81	Preparation and characterization of anticancer niosomal withaferinâ€“A formulation for improved delivery to cancer cells: In vitro, in vivo, and in silico evaluation. Journal of Drug Delivery Science and Technology, 2020, 59, 101863.	1.4	15
82	Structural Basis of Binding and Rationale for the Potent Urease Inhibitory Activity of Biscoumarins. BioMed Research International, 2014, 2014, 1-12.	0.9	14
83	Synthesis, molecular structure, spectral analysis, and biological activity of new malonamide derivatives as Î±-glucosidase inhibitors. Journal of Molecular Structure, 2017, 1134, 253-264.	1.8	14
84	Benzylidine indane-1,3-diones: As novel urease inhibitors; synthesis, in vitro, and in silico studies. Bioorganic Chemistry, 2018, 81, 658-671.	2.0	14
85	Pharmacophore model-based virtual screening, docking, biological evaluation and molecular dynamics simulations for inhibitors discovery against Î±-tryptophan synthase from Mycobacterium tuberculosis. Journal of Biomolecular Structure and Dynamics, 2021, 39, 610-620.	2.0	14
86	Isatin thiazoles as antidiabetic: Synthesis, in vitro enzyme inhibitory activities, kinetics, and in silico studies. Archiv Der Pharmazie, 2022, 355, e2100481.	2.1	14
87	In silico studies of urease inhibitors to explore ligand-enzyme interactions. Journal of Enzyme Inhibition and Medicinal Chemistry, 2009, 24, 151-156.	2.5	13
88	Synthesis and QSAR analysis of chalcone derivatives as nitric oxide inhibitory agent. Medicinal Chemistry Research, 2012, 21, 1953-1966.	1.1	13
89	Reprofiling of fullâ€length phosphonated carbocyclic 2â€²â€oxaâ€3â€²â€azaâ€nucleosides toward antiproliferative agents: Synthesis, antiproliferative activity, and molecular docking study. Chemical Biology and Drug Design, 2017, 90, 679-689.	1.5	13
90	Tambulin from Zanthoxylum armatum acutely potentiates the glucose-induced insulin secretion via KATP-independent Ca2+-dependent amplifying pathway. Biomedicine and Pharmacotherapy, 2019, 120, 109348.	2.5	13

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91	Molecular dynamics simulations reveal structural insights into inhibitor binding modes and mechanism of casein kinase II inhibitors. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1120-1135.	2.0	13
92	Docking and 3D-QSAR modeling of cyclin-dependent kinase 5/p25 inhibitors. Journal of Molecular Modeling, 2011, 17, 1149-1161.	0.8	12
93	The exploration of interaction studies of smaller size, mostly ignored yet intrinsically inestimable molecules towards BSA; An example of STD and DOSY NMR. Open Chemistry, 2014, 12, 332-340.	1.0	12
94	In-silico identification of the binding mode of synthesized adamantyl derivatives inside cholinesterase enzymes. Acta Pharmacologica Sinica, 2015, 36, 879-886.	2.8	12
95	3D-QSAR Studies on Barbituric Acid Derivatives as Urease Inhibitors and the Effect of Charges on the Quality of a Model. International Journal of Molecular Sciences, 2016, 17, 657.	1.8	12
96	Pharmacologically Safe Nanomicelles of Amphotericin B With Lipids: Nuclear Magnetic Resonance and Molecular Docking Approach. Journal of Pharmaceutical Sciences, 2017, 106, 3574-3582.	1.6	12
97	Analyzing the Behavior of Neuronal Pathways in Alzheimer's Disease Using Petri Net Modeling Approach. Frontiers in Neuroinformatics, 2018, 12, 26.	1.3	12
98	Peptide conjugates of 18Î²-glycyrrhetinic acid as potent inhibitors of Î±-glucosidase and AGEs-induced oxidation. European Journal of Pharmaceutical Sciences, 2022, 168, 106045.	1.9	12
99	Deciphering the Impact of Mutations on the Binding Efficacy of SARS-CoV-2 Omicron and Delta Variants With Human ACE2 Receptor. Frontiers in Chemistry, 0, 10, .	1.8	12
100	In silico studies on 2,3-dihydro-1,5-benzothiazepines as cholinesterase inhibitors. Medicinal Chemistry Research, 2012, 21, 2329-2339.	1.1	11
101	In vitro and in silico exploration of IL-2 inhibition by small drug-like molecules. Medicinal Chemistry Research, 2013, 22, 5739-5751.	1.1	11
102	A combined 3D-QSAR and docking studies for the In-silicoprediction of HIV-protease inhibitors. Chemistry Central Journal, 2013, 7, 88.	2.6	11
103	Exploring Novel N-Myristoyltransferase Inhibitors: A Molecular Dynamics Simulation Approach. ACS Omega, 2019, 4, 13658-13670.	1.6	11
104	Re-purposing of hepatitis C virus FDA approved direct acting antivirals as potential SARS-CoV-2 protease inhibitors. Journal of Molecular Structure, 2022, 1250, 131920.	1.8	11
105	Immunoinformatic approach for the construction of multi-epitopes vaccine against omicron COVID-19 variant. Virology, 2022, 572, 28-43.	1.1	11
106	3D Structure Prediction of Human Î²1-Adrenergic Receptor via Threading-Based Homology Modeling for Implications in Structure-Based Drug Designing. PLoS ONE, 2015, 10, e0122223.	1.1	10
107	Insulin releasing effect of some pure compounds from Moringa oleifera on mice islets. Medicinal Chemistry Research, 2018, 27, 1408-1418.	1.1	10
108	Computational and biological characterization of fusion proteins of two insecticidal proteins for control of insect pests. Scientific Reports, 2018, 8, 4837.	1.6	10

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109	Characterization of the interactions between coumarin-derivatives and acetylcholinesterase: Examination by NMR and docking simulations. Journal of Molecular Modeling, 2018, 24, 207.	0.8	10
110	Degradation kinetics of fluvoxamine in buffer solutions: In silico ADMET profiling and identification of degradation products by LC-MS/ESI. Arabian Journal of Chemistry, 2020, 13, 4134-4146.	2.3	10
111	Inhibitory Effects of Myrtucommuacetalone 1 (MCA-1) from Myrtus Communis on Inflammatory Response in Mouse Macrophages. Molecules, 2020, 25, 13.	1.7	10
112	Potential of sodium deoxycholate sulfate as a carrier for polymyxin B: Physicochemical properties, bioactivity and in vitro safety. Journal of Drug Delivery Science and Technology, 2020, 58, 101779.	1.4	10
113	Phenylpyrazalopyrimidines as Tyrosine Kinase Inhibitors: Synthesis, Antiproliferative Activity, and Molecular Simulations. Molecules, 2020, 25, 2135.	1.7	10
114	Active site characterization and structure based 3D-QSAR studies on non-redox type 5-lipoxygenase inhibitors. European Journal of Pharmaceutical Sciences, 2016, 88, 26-36.	1.9	9
115	In-silico designing and characterization of binding modes of two novel inhibitors for CB1 receptor against obesity by classical 3D-QSAR approach. Journal of Molecular Graphics and Modelling, 2019, 89, 199-214.	1.3	9
116	An investigation of the kinetic and anti-angiogenic properties of plant glycoside inhibitors of thymidine phosphorylase. Journal of Asian Natural Products Research, 2009, 11, 159-167.	0.7	8
117	A Novel Pharmacophore Model to Identify Leads for Simultaneous Inhibition of Antiâ€coagulation and Antiâ€inflammatory Activities of Snake Venom Phospholipase A₂. Chemical Biology and Drug Design, 2012, 79, 431-441.	1.5	8
118	Molecular docking simulation studies on potent butyrylcholinesterase inhibitors obtained from microbial transformation of dihydrotestosterone. Chemistry Central Journal, 2013, 7, 164.	2.6	8
119	Crude to leads: a triple-pronged direct NMR approach in coordination with docking simulation. Analyst, The, 2013, 138, 5137.	1.7	8
120	Development of robust QSAR model using rapid overlay of crystal structures (ROCS) based alignment: a test case of Tubulin inhibitors. Medicinal Chemistry Research, 2013, 22, 3229-3241.	1.1	8
121	4-Benzyloxylonchocarpin and Muracatanes A-C from Ranunculus muricatus L. and Their Biological Effects. Biomolecules, 2020, 10, 1562.	1.8	8
122	Novel 4,6-Disubstituted s-Triazin-2-yl Amino Acid Derivatives as Promising Antifungal Agents. Journal of Fungi (Basel, Switzerland), 2020, 6, 237.	1.5	8
123	Benzilydene and thiourea derivatives as new classes of carbonic anhydrase inhibitors: an in vitro and molecular docking study. Medicinal Chemistry Research, 2021, 30, 552-563.	1.1	8
124	Probing CAS database as prospective antiviral agents against SARS-CoV-2 main protease. Journal of Molecular Structure, 2021, 1231, 129953.	1.8	8
125	Aryl hydrazones linked thiazolyl coumarin hybrids as potential urease inhibitors. Journal of the Iranian Chemical Society, 2022, 19, 1221-1238.	1.2	8
126	Isolation of Cardamonin and Pinostrobin Chalcone from the Rhizomes of Boesenbergia rotunda (L.) Mansf. and their Cytotoxic Effects on H-29 and MDA-MB-231 Cancer Cell Lines. Natural Products Journal, 2019, 9, 341-348.	0.1	8

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127	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
128	Protein kinase A-dependent insulinotropic effect of selected flavonoids. International Journal of Biological Macromolecules, 2018, 119, 149-156.	3.6	7
129	Characterization of cryptic allosteric site at IL-4RÎ±: New paradigm towards IL-4/IL-4R inhibition. International Journal of Biological Macromolecules, 2019, 123, 239-245.	3.6	7
130	Discovery of Potential Chemical Probe as Inhibitors of CXCL12 Using Ligand-Based Virtual Screening and Molecular Dynamic Simulation. Molecules, 2020, 25, 4829.	1.7	7
131	Insights into the molecular basis of acetylcholinesterase inhibition by xanthones: an integrative in silico and in vitro approach. Molecular Simulation, 2020, 46, 253-261.	0.9	7
132	Effect of sodium deoxycholate sulfate on outer membrane permeability and neutralization of bacterial lipopolysaccharides by polymyxin B formulations. International Journal of Pharmaceutics, 2020, 581, 119265.	2.6	7
133	Amphiphilic desmuramyl peptides for the rational design of new vaccine adjuvants: Synthesis, inÂvitro modulation of inflammatory response and molecular docking studies. European Journal of Medicinal Chemistry, 2021, 209, 112863.	2.6	7
134	Synthesis of Highly Potent Anti-Inflammatory Compounds (ROS Inhibitors) from Isonicotinic Acid. Molecules, 2021, 26, 1272.	1.7	7
135	Molecular docking study on columbin isolated from Tinospora cordifolia as a cholinesterase inhibitor. Tropical Journal of Pharmaceutical Research, 2022, 20, 337-343.	0.2	7
136	3D-QSPR Method of Computational Technique Applied on Red Reactive Dyes by Using CoMFA Strategy. International Journal of Molecular Sciences, 2011, 12, 8862-8877.	1.8	6
137	A combined 3D-QSAR and molecular docking strategy to understand the binding mechanism of V600EB-RAF inhibitors. Molecular Diversity, 2012, 16, 771-785.	2.1	6
138	Structure-based 3D-QSAR models and dynamics analysis of novel N-benzyl pyridinone as p38Î± MAP kinase inhibitors for anticytokine activity. Journal of Molecular Graphics and Modelling, 2012, 36, 48-61.	1.3	6
139	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
140	Atom and receptor based 3D QSAR models for generating new conformations from pyrazolopyrimidine as IL-2 inducible tyrosine kinase inhibitors. Journal of Molecular Graphics and Modelling, 2017, 74, 379-395.	1.3	6
141	Dithiocarbamate derivatives inhibit Î±â€glucosidase through an apparent allosteric site on the enzyme. Chemical Biology and Drug Design, 2021, 98, 283-294.	1.5	6
142	Exploration of the structural requirements of Aurora Kinase B inhibitors by a combined QSAR, modelling and molecular simulation approach. Scientific Reports, 2021, 11, 18707.	1.6	6
143	Optimization of Structure Based Virtual Screening Protocols Against Thymidine Monophosphate Kinase Inhibitors as Antitubercular Agents. Molecular Informatics, 2011, 30, 851-862.	1.4	5
144	In-vitro immunomodulatory and anti-cancerous activities of biotransformed products of Dianabol through Azadirachta indica and its molecular docking studies. Chemistry Central Journal, 2013, 7, 163.	2.6	5

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145	Bioinformatics: A rational combine approach used for the identification and in-vitro activity evaluation of potent Î²-Glucuronidase inhibitors. PLoS ONE, 2018, 13, e0200502.	1.1	5
146	Quantum mechanics and 3D-QSAR studies on thienopyridine analogues: inhibitors of IKKÎ². Heliyon, 2020, 6, e04125.	1.4	5
147	Enamine Barbiturates and Thiobarbiturates as a New Class of Bacterial Urease Inhibitors. Applied Sciences (Switzerland), 2020, 10, 3523.	1.3	5
148	Template-based structure prediction and molecular dynamics simulation study of two mammalian Aspartyl-tRNA synthetases. Journal of Molecular Graphics and Modelling, 2010, 28, 401-412.	1.3	4
149	Dynamic changes in the secondary structure of ECE-1 and XCE account for their different substrate specificities. BMC Bioinformatics, 2012, 13, 285.	1.2	4
150	Molecular dynamics simulation of interleukin-2 and its complex and determination of the binding free energy. Molecular Simulation, 2018, 44, 1411-1425.	0.9	4
151	Structural insight into TNF-Î± inhibitors through combining pharmacophore-based virtual screening and molecular dynamic simulation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 5920-5939.	2.0	4
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