Zaheer Ul-Haq

List of Publications by Citations

184 papers	2,690 citations	27 h-index	42 g-index
196 ext. papers	3,213 ext. citations	3.6 avg, IF	5.49 L-index

#	Paper	IF	Citations
184	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, 5200-7	6.8	222
183	Identification of chymotrypsin-like protease inhibitors of SARS-CoV-2 integrated computational approach. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 2607-2616	3.6	143
182	Synthesis of novel inhibitors of β-glucuronidase based on benzothiazole skeleton and study of their binding affinity by molecular docking. *Bioorganic and Medicinal Chemistry*, **2011**, 19, 4286-94	3.4	84
181	Docking based 3D-QSAR studies applied at the BRAF inhibitors to understand the binding mechanism. *Journal of Cheminformatics*, **2012**, 4,	8.6	78
180	Withanolides, a new class of natural cholinesterase inhibitors with calcium antagonistic properties. *Biochemical and Biophysical Research Communications*, **2005**, 334, 276-87	3.4	73
179	Juliflorine: a potent natural peripheral anionic-site-binding inhibitor of acetylcholinesterase with calcium-channel blocking potential, a leading candidate for Alzheimer's disease therapy. *Biochemical and Biophysical Research Communications*, **2005**, 332, 1171-7	3.4	67
178	Identification of novel urease inhibitors by high-throughput virtual and in vitro screening. *ACS Medicinal Chemistry Letters*, **2010**, 1, 145-9	4.3	58
177	Presence of antispasmodic, antidiarrheal, antisecretory, calcium antagonist and acetylcholinesterase inhibitory steroidal alkaloids in Sarcococca saligna. *Planta Medica*, **2005**, 71, 120-5	3.1	49
176	Biological and molecular docking studies on coagulin-H: Human IL-2 novel natural inhibitor. *Molecular Immunology*, **2006**, 43, 1855-63	4.3	48
175	Interleukin-4 receptor signaling and its binding mechanism: A therapeutic insight from inhibitors tool box. *Cytokine and Growth Factor Reviews*, **2016**, 32, 3-15	17.9	45
174	BRAF gene: From human cancers to developmental syndromes. *Saudi Journal of Biological Sciences*, **2015**, 22, 359-73	4	44
173	Kinetics and structure-activity relationship studies on pregnane-type steroidal alkaloids that inhibit cholinesterases. *Bioorganic and Medicinal Chemistry*, **2004**, 12, 1995-2003	3.4	42
172	Pregnane-Type Steroidal Alkaloids of Sarcococca saligna: a New Class of Cholinesterase Inhibitors. *Helvetica Chimica Acta*, **2002**, 85, 678-688	2	36
171	Molecular docking studies of natural cholinesterase-inhibiting steroidal alkaloids from Sarcococca saligna. *Journal of Medicinal Chemistry*, **2003**, 46, 5087-90	8.3	36
170	Synthesis of pyrimidine-2,4,6-trione derivatives: Anti-oxidant, anti-cancer, β-glucosidase, β-glucuronidase inhibition and their molecular docking studies. *Bioorganic Chemistry*, **2016**, 68, 72-9	5.1	35
169	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, 1092-103	6.1	35
168	New Cholinesterase-Inhibiting Steroidal Alkaloids from Sarcococca saligna. *Helvetica Chimica Acta*, **2004**, 87, 439-448	2	35

167	□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	5.1	34
166	Molecular modeling-based antioxidant arylidene barbiturates as urease inhibitors. *Journal of Molecular Graphics and Modelling*, **2011**, 30, 153-6	2.8	34
165	New pregnane-type steroidal alkaloids from Sarcocca saligna and their cholinesterase inhibitory activity. *Steroids*, **2004**, 69, 735-41	2.8	34
164	Cholinesterase inhibitory and spasmolytic potential of steroidal alkaloids. *Journal of Steroid Biochemistry and Molecular Biology*, **2004**, 92, 477-84	5.1	34
163	Identification of potent urease inhibitors via ligand- and structure-based virtual screening and in vitro assays. *Journal of Molecular Graphics and Modelling*, **2010**, 28, 792-8	2.8	33
162	Synthesis and biological activity of oxadiazole and triazolothiadiazole derivatives as tyrosinase inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 3755-9	2.9	32
161	Structure-based design, synthesis and biological evaluation of □glucuronidase inhibitors. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 577-85	4.2	30
160	3D-QSAR CoMFA studies on bis-coumarine analogues as urease inhibitors: a strategic design in anti-urease agents. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 3456-61	3.4	30
159	3D-QSAR studies on natural acetylcholinesterase inhibitors of Sarcococca saligna by comparative molecular field analysis (CoMFA). *Bioorganic and Medicinal Chemistry Letters*, **2003**, 13, 4375-80	2.9	29
158	Design and synthesis of chalcone derivatives as potent tyrosinase inhibitors and their structural activity relationship. *Journal of Molecular Structure*, **2015**, 1085, 97-103	3.4	28
157	Classical and QM/MM MD simulations of sodium(I) and potassium(I) ions in aqueous solution. *Journal of Molecular Liquids*, **2010**, 153, 95-100	6	27
156	Structure based virtual screening-driven identification of monastrol as a potent urease inhibitor. *Journal of Molecular Graphics and Modelling*, **2013**, 43, 47-57	2.8	25
155	Eriodictyol stimulates insulin secretion through cAMP/PKA signaling pathway in mice islets. *European Journal of Pharmacology*, **2018**, 820, 245-255	5.3	25
154	In silico and in vitro immunomodulatory studies on compounds of Lindelofia stylosa. *Chemical Biology and Drug Design*, **2012**, 79, 290-9	2.9	24
153	5-Acetyl-6-methyl-4-aryl-3,4-dihydropyrimidin-2(1H)-ones: As potent urease inhibitors; synthesis, in vitro screening, and molecular modeling study. *Bioorganic Chemistry*, **2018**, 76, 37-52	5.1	23
152	Immunosuppressive activity of buxidin and E-buxenone from Buxus hyrcana. *Chemical Biology and Drug Design*, **2010**, 75, 310-7	2.9	23
151	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, 21-8	5.1	22
150	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	4.2	20

149	Benchmarking docking and scoring protocol for the identification of potential acetylcholinesterase inhibitors. *Journal of Molecular Graphics and Modelling*, **2010**, 28, 870-82	2.8	20
148	In silico modeling of the specific inhibitory potential of thiophene-2,3-dihydro-1,5-benzothiazepine against BChE in the formation of beta-amyloid plaques associated with Alzheimer's disease. *Theoretical Biology and Medical Modelling*, **2010**, 7, 22	2.3	20
147	Catalytic asymmetric synthesis of indole derivatives as novel -glucosidase inhibitors in vitro. *Bioorganic Chemistry*, **2018**, 79, 350-354	5.1	20
146	Synthesis and dynamics studies of barbituric acid derivatives as urease inhibitors. *Chemistry Central Journal*, **2015**, 9, 63		19
145	Synthesis, antimicrobial activity, pharmacophore modeling and molecular docking studies of new pyrazole-dimedone hybrid architectures. *Chemistry Central Journal*, **2018**, 12, 29		19
144	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, 202-10	2.8	19
143	Synthesis of thiobarbituric acid derivatives: In vitro -glucosidase inhibition and molecular docking studies. *Bioorganic Chemistry*, **2017**, 75, 99-105	5.1	19
142	Molecular docking studies of potent inhibitors of tyrosinase and -glucosidase. *Medicinal Chemistry Research*, **2012**, 21, 1677-1683	2.2	19
141	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	3.7	19
140	Synthesis, and In Vitro and In Silico -Glucosidase Inhibitory Studies of 5-Chloro-2-Aryl Benzo[d]thiazoles. *Bioorganic Chemistry*, **2018**, 78, 269-279	5.1	18
139	Synthesis, bioactivity, molecular docking and POM analyses of novel substituted thieno[2,3-b]thiophenes and related congeners. *Molecules*, **2015**, 20, 1824-41	4.8	18
138	First comprehensive in silico analysis of the functional and structural consequences of SNPs in human GalNAc-T1 gene. *Computational and Mathematical Methods in Medicine*, **2014**, 2014, 904052	2.8	18
137	Family 18 chitolectins: comparison of MGP40 and HUMGP39. *Biochemical and Biophysical Research Communications*, **2007**, 359, 221-6	3.4	18
136	Indole acrylonitriles as potential anti-hyperglycemic agents: Synthesis, -glucosidase inhibitory activity and molecular docking studies. *Bioorganic and Medicinal Chemistry*, **2020**, 28, 115605	3.4	18
135	Identification of novel Interleukin-2 inhibitors through computational approaches. *Molecular Diversity*, **2013**, 17, 345-55	3.1	17
134	Successful computer guided planned synthesis of (4R)-thiazolidine carboxylic acid and its 2-substituted analogues as urease inhibitors. *Molecular Diversity*, **2006**, 10, 223-31	3.1	16
133	Synthesis of azachalcones, their -amylase, -glucosidase inhibitory activities, kinetics, and molecular docking studies. *Bioorganic Chemistry*, **2021**, 106, 104489	5.1	16
132	Natural flavonoid -glucosidase inhibitors from Retama raetam: Enzyme inhibition and molecular docking reveal important interactions with the enzyme active site. *Bioorganic Chemistry*, **2019**, 87, 736-742	5.1	15

131	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	5	15
130	In silico identification of novel inhibitors against Plasmodium falciparum dihydroorate dehydrogenase. *Journal of Molecular Graphics and Modelling*, **2013**, 40, 40-7	2.8	15
129	Ligand-based 3D-QSAR studies of physostigmine analogues as acetylcholinesterase inhibitors. *Chemical Biology and Drug Design*, **2009**, 74, 571-81	2.9	15
128	CoMFA and CoMSIA 3D-QSAR analysis on hydroxamic acid derivatives as urease inhibitors. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2009**, 24, 272-8	5.6	15
127	Synthesis, anti-microbial and molecular docking studies of quinazolin-4(3H)-one derivatives. *Molecules*, **2014**, 19, 8725-39	4.8	14
126	Combined pharmacophore and 3D-QSAR study on a series of Staphylococcus aureus Sortase A inhibitors. *Chemical Biology and Drug Design*, **2012**, 80, 300-14	2.9	14
125	Molecular dynamics simulation of mammalian 15S-lipoxygenase with AMBER force field. *European Biophysics Journal*, **2011**, 40, 715-26	1.9	14
124	Coumarin derivatives as acetyl- and butyrylcholinestrase inhibitors: An in□vitro, molecular docking, and molecular dynamics simulations study. *Heliyon*, **2019**, 5, e01552	3.6	13
123	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	7.5	12
122	Synthesis and characterisation of thiobarbituric acid enamine derivatives, and evaluation of their □glucosidase inhibitory and anti-glycation activity. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2020**, 35, 692-701	5.6	12
121	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	4.4	12
120	Synthesis and QSAR analysis of chalcone derivatives as nitric oxide inhibitory agent. *Medicinal Chemistry Research*, **2012**, 21, 1953-1966	2.2	12
119	Superoxide Scavenging and Antiglycation Activity of Rhinacanthins-rich Extract Obtained from the Leaves of. *Pharmacognosy Magazine*, **2017**, 13, 652-658	0.8	12
118	Synthetic flavonoids as potential antiviral agents against SARS-CoV-2 main protease. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-12	3.6	12
117	Reprofiling of full-length phosphonated carbocyclic 2'-oxa-3'-aza-nucleosides toward antiproliferative agents: Synthesis, antiproliferative activity, and molecular docking study. *Chemical Biology and Drug Design*, **2017**, 90, 679-689	2.9	11
116	Synthesis, molecular structure, spectral analysis, and biological activity of new malonamide derivatives as □glucosidase inhibitors. *Journal of Molecular Structure*, **2017**, 1134, 253-264	3.4	11
115	In-silico identification of the binding mode of synthesized adamantyl derivatives inside cholinesterase enzymes. *Acta Pharmacologica Sinica*, **2015**, 36, 879-86	8	11
114	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	5	11

113	Development of sulfonamide-based Schiff bases targeting urease inhibition: Synthesis, characterization, inhibitory activity assessment, molecular docking and ADME studies. *Bioorganic Chemistry*, **2020**, 102, 104057	5.1	11
112	Bioactivity, Safety, and Efficacy of Amphotericin B Nanomicellar Aerosols Using Sodium Deoxycholate Sulfate as the Lipid Carrier. *AAPS PharmSciTech*, **2018**, 19, 2077-2086	3.9	11
111	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,	4.8	11
110	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	3.7	11
109	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	1.6	11
108	An in-silico evaluation of COVID-19 main protease with clinically approved drugs. *Journal of Molecular Graphics and Modelling*, **2020**, 101, 107758	2.8	11
107	Preparation and characterization of anticancer niosomal withaferin 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	4.5	10
106	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, 3000-8	3.4	10
105	In vitro and in silico exploration of IL-2 inhibition by small drug-like molecules. *Medicinal Chemistry Research*, **2013**, 22, 5739-5751	2.2	10
104	3D structure prediction of human 1-adrenergic receptor via threading-based homology modeling for implications in structure-based drug designing. *PLoS ONE*, **2015**, 10, e0122223	3.7	10
103	In silico studies on 2,3-dihydro-1,5-benzothiazepines as cholinesterase inhibitors. *Medicinal Chemistry Research*, **2012**, 21, 2329-2339	2.2	10
102	In silico studies of urease inhibitors to explore ligand-enzyme interactions. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2009**, 24, 151-6	5.6	10
101	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,	6.3	10
100	Synthesis of Oxindole Analogues, Biological Activity, and In Silico Studies. *ChemistrySelect*, **2019**, 4, 10510-10516	2.8	9
99	Purification and Characterization of a Nonspecific Lipid Transfer Protein 1 (nsLTP1) from Ajwain (Trachyspermum ammi) Seeds. *Scientific Reports*, **2019**, 9, 4148	4.9	9
98	Analyzing the Behavior of Neuronal Pathways in Alzheimer's Disease Using Petri Net Modeling Approach. *Frontiers in Neuroinformatics*, **2018**, 12, 26	3.9	9
97	Structural basis of binding and rationale for the potent urease inhibitory activity of biscoumarins. *BioMed Research International*, **2014**, 2014, 935039	3	9
96	A combined 3D-QSAR and docking studies for the In-silico prediction of HIV-protease inhibitors. *Chemistry Central Journal*, **2013**, 7, 88		9

95	Docking and 3D-QSAR modeling of cyclin-dependent kinase 5/p25 inhibitors. *Journal of Molecular Modeling*, **2011**, 17, 1149-61	2	9
94	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	2.7	9
93	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	3.6	9
92	Insulin releasing effect of some pure compounds from Moringa oleifera on mice islets. *Medicinal Chemistry Research*, **2018**, 27, 1408-1418	2.2	8
91	Pharmacologically Safe Nanomicelles of Amphotericin B With Lipids: Nuclear Magnetic Resonance and Molecular Docking Approach. *Journal of Pharmaceutical Sciences*, **2017**, 106, 3574-3582	3.9	8
90	Brine shrimp lethality assay 'an effective prescreen': microwave-assisted synthesis, BSL toxicity and 3DQSAR studies-based designing, docking and antitumor evaluation of potent chalcones. *Pharmaceutical Biology*, **2013**, 51, 1091-103	3.8	8
89	Synthesis of a New Class of Spirooxindole-Benzo[]Thiophene-Based Molecules as Acetylcholinesterase Inhibitors. *Molecules*, **2020**, 25,	4.8	8
88	Identification of potential TNF-□nhibitors: from in silico to in vitro studies. *Scientific Reports*, **2020**, 10, 20974	4.9	8
87	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	5.1	8
86	Insights into the molecular basis of acetylcholinesterase inhibition by xanthones: an integrative in silico and in vitro approach. *Molecular Simulation*, **2020**, 46, 253-261	2	7
85	Characterization of the interactions between coumarin-derivatives and acetylcholinesterase: Examination by NMR and docking simulations. *Journal of Molecular Modeling*, **2018**, 24, 207	2	7
84	A novel pharmacophore model to identify leads for simultaneous inhibition of anti-coagulation and anti-inflammatory activities of snake venom phospholipase A(2). *Chemical Biology and Drug Design*, **2012**, 79, 431-41	2.9	7
83	Molecular docking simulation studies on potent butyrylcholinesterase inhibitors obtained from microbial transformation of dihydrotestosterone. *Chemistry Central Journal*, **2013**, 7, 164		7
82	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	2.2	7
81	Biology-oriented drug synthesis (BIODS), in vitro urease inhibitory activity, and in silico studies on ibuprofen derivatives. *Molecular Diversity*, **2021**, 25, 143-157	3.1	7
80	Pharmacophore model-based virtual screening, docking, biological evaluation and molecular dynamics simulations for inhibitors discovery against -tryptophan synthase from. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 610-620	3.6	7
79	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	2.8	6
78	Phenylpyrazalopyrimidines as Tyrosine Kinase Inhibitors: Synthesis, Antiproliferative Activity, and Molecular Simulations. *Molecules*, **2020**, 25,	4.8	6

77	Structure-based 3D-QSAR models and dynamics analysis of novel N-benzyl pyridinone as p38 MAP kinase inhibitors for anticytokine activity. *Journal of Molecular Graphics and Modelling*, **2012**, 36, 48-61	2.8	6
76	Crude to leads: a triple-pronged direct NMR approach in coordination with docking simulation. *Analyst, The*, **2013**, 138, 5137-45	5	6
75	An investigation of the kinetic and anti-angiogenic properties of plant glycoside inhibitors of thymidine phosphorylase. *Journal of Asian Natural Products Research*, **2009**, 11, 159-67	1.5	6
74	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	0.6	6
73	Benzylidine indane-1,3-diones: As novel urease inhibitors; synthesis, in vitro, and in silico studies. *Bioorganic Chemistry*, **2018**, 81, 658-671	5.1	6
72	Computational and biological characterization of fusion proteins of two insecticidal proteins for control of insect pests. *Scientific Reports*, **2018**, 8, 4837	4.9	5
71	A combined 3D-QSAR and molecular docking strategy to understand the binding mechanism of (V600E)B-RAF inhibitors. *Molecular Diversity*, **2012**, 16, 771-85	3.1	5
70	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		5
69	Optimization of Structure Based Virtual Screening Protocols Against Thymidine Monophosphate Kinase Inhibitors as Antitubercular Agents. *Molecular Informatics*, **2011**, 30, 851-62	3.8	5
68	3D-QSPR method of computational technique applied on red reactive dyes by using CoMFA strategy. *International Journal of Molecular Sciences*, **2011**, 12, 8862-77	6.3	5
67	Characterization of cryptic allosteric site at IL-4R New paradigm towards IL-4/IL-4R inhibition. *International Journal of Biological Macromolecules*, **2019**, 123, 239-245	7.9	5
66	Amphiphilic desmuramyl peptides for the rational design of new vaccine adjuvants: Synthesis, in vitro modulation of inflammatory response and molecular docking studies. *European Journal of Medicinal Chemistry*, **2021**, 209, 112863	6.8	5
65	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	2.8	4
64	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	4.5	4
63	Exploring Novel -Myristoyltransferase Inhibitors: A Molecular Dynamics Simulation Approach. *ACS Omega*, **2019**, 4, 13658-13670	3.9	4
62	Three-dimensional quantitative structure ctivity relationship (CoMSIA) analysis of bis-coumerine analogues as urease inhibitors. *Medicinal Chemistry Research*, **2013**, 22, 498-504	2.2	4
61	Dynamic changes in the secondary structure of ECE-1 and XCE account for their different substrate specificities. *BMC Bioinformatics*, **2012**, 13, 285	3.6	4
60	Template-based structure prediction and molecular dynamics simulation study of two mammalian Aspartyl-tRNA synthetases. *Journal of Molecular Graphics and Modelling*, **2010**, 28, 401-12	2.8	4

59	2-Mercapto Benzothiazole Derivatives: As Potential Leads for the Diabetic Management. *Medicinal Chemistry*, **2020**, 16, 826-840	1.8	4
58	Prediction of Binding Affinities for Hydroxamic Acid Derivatives as Urease Inhibitors by Molecular Docking and 3D-QSAR Studies. *Letters in Drug Design and Discovery*, **2009**, 6, 93-100	0.8	4
57	Novel 4,6-Disubstituted -Triazin-2-yl Amino Acid Derivatives as Promising Antifungal Agents. *Journal of Fungi (Basel, Switzerland)*, **2020**, 6,	5.6	4
56	Bioinformatics: A rational combine approach used for the identification and in-vitro activity evaluation of potent Glucuronidase inhibitors. *PLoS ONE*, **2018**, 13, e0200502	3.7	4
55	Molecular dynamics simulation of interleukin-2 and its complex and determination of the binding free energy. *Molecular Simulation*, **2018**, 44, 1411-1425	2	4
54	Anti-diarrheal activities of phytol along with its possible mechanism of action through in-vivo and in-silico models. *Cellular and Molecular Biology*, **2020**, 66, 243	1.1	3
53	In-silico analysis of chromone containing sulfonamide derivatives as human carbonic anhydrase inhibitors. *Medicinal Chemistry*, **2013**, 9, 608-16	1.8	3
52	Quantum mechanics and 3D-QSAR studies on thienopyridine analogues: inhibitors of IKK *Heliyon*, **2020**, 6, e04125	3.6	3
51	Discovery of Potential Chemical Probe as Inhibitors of CXCL12 Using Ligand-Based Virtual Screening and Molecular Dynamic Simulation. *Molecules*, **2020**, 25,	4.8	3
50	Probing CAS database as prospective antiviral agents against SARS-CoV-2 main protease. *Journal of Molecular Structure*, **2021**, 1231, 129953	3.4	3
49	Synthesis of Highly Potent Anti-Inflammatory Compounds (ROS Inhibitors) from Isonicotinic Acid. *Molecules*, **2021**, 26,	4.8	3
48	Exploration of the structural requirements of Aurora Kinase B inhibitors by a combined QSAR, modelling and molecular simulation approach. *Scientific Reports*, **2021**, 11, 18707	4.9	3
47	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	2.8	2
46	Tambulin from Zanthoxylum armatum acutely potentiates the glucose-induced insulin secretion via K-independent Ca-dependent amplifying pathway. *Biomedicine and Pharmacotherapy*, **2019**, 120, 109348	7.5	2
45	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	6.5	2
44	Protein kinase A-dependent insulinotropic effect of selected flavonoids. *International Journal of Biological Macromolecules*, **2018**, 119, 149-156	7.9	2
43	Ligand-based 3D-QSAR studies of diaryl acyl-sulfonamide analogues as human umbilical vein endothelial cells inhibitors stimulated by VEGF. *Chemical Biology and Drug Design*, **2011**, 77, 288-94	2.9	2
42	Molecular dynamics simulation of Axillaridine-A: a potent natural cholinesterase inhibitor. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2009**, 24, 1101-5	5.6	2

41	Re-Purposing of Hepatitis C Virus FDA Approved Direct Acting Antivirals as Potential SARS-CoV-2 Protease Inhibitors. *Journal of Molecular Structure*, **2021**, 131920	3.4	2
40	Peptide conjugates of 18□glycyrrhetinic acid as potent inhibitors of □glucosidase and AGEs-induced oxidation. *European Journal of Pharmaceutical Sciences*, **2021**, 168, 106045	5.1	2
39	Relative assessment of different statistical instruments and measures for the prediction of promising outcomes using docking, virtual screening and ADMET analysis against HIV-RT. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-13	3.6	2
38	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	5.9	2
37	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	2.2	2
36	Deciphering the Role of PKC in Calpain-CAST System Through Formal Modeling Approach. *Lecture Notes in Computer Science*, **2019**, 60-71	0.9	1
35	Probing the mechanism of peptide binding to REV response element RNA of HIV-1; MD simulations and free energy calculations. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-10	3.6	1
34	In silico based investigation of dynamic variations in neprilysin (NEP and NEP2) proteins for extracting the point of specificity. *Molecular BioSystems*, **2016**, 12, 1024-36		1
33	Molecular docking- and genetic algorithm-based approaches to produce robust 3D-QSAR models. *Medicinal Chemistry Research*, **2014**, 23, 2198-2206	2.2	1
32	CoMFA and CoMSIA studies on a series of fluroquinolone derivatives for potential anti-inflammatory activity. *Analytical Methods*, **2014**, 6, 6823	3.2	1
31	Gd-Complexes of New Arylpiperazinyl Conjugates of DTPA-Bis(amides): Synthesis, Characterization and Magnetic Relaxation Properties. *Molecules*, **2015**, 20, 7807-19	4.8	1
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