Zaheer Ul-Haq

List of Publications by Year in Descending Order

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	Isatin thiazoles as antidiabetic: Synthesis, in vitro enzyme inhibitory activities, kinetics, and in silico studies.. *Archiv Der Pharmazie*, **2022**, e2100481	4.3	0
183	Immunoinformatic approach for the construction of multi-epitopes vaccine against omicron COVID-19 variant.. *Virology*, **2022**, 572, 28-43	3.6	1
182	Sarcorucinine-D Inhibits Cholinesterases and Calcium Channels: Molecular Dynamics Simulation and In Vitro Mechanistic Investigations. *Molecules*, **2022**, 27, 3361	4.8	0
181	In silico data mining of large-scale databases for the virtual screening of human interleukin-2 inhibitors. *Acta Pharmaceutica*, **2021**, 71, 33-56	3.2	
180	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
179	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
178	Theoretical investigation of selective ligand binding mode of galanin receptors. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-11	3.6	0
177	Structural insight into TNF- inhibitors through combining pharmacophore-based virtual screening and molecular dynamic simulation. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 5920-5939	3.6	1
176	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
175	Exploring the Molecular Mechanisms of 17-HSD5-induced Carcinogenicity of Catha edulis via Molecular Modeling Approach. *Medicinal Chemistry*, **2021**, 17, 418-428	1.8	
174	Site-directed Fragnomics and MD Simulations Approaches to Identify Interleukin-2 Inhibitors. *Medicinal Chemistry*, **2021**, 17, 407-417	1.8	
173	Characterization of the multidrug efflux transporter styMdtM from Salmonella enterica serovar Typhi. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 1193-1204	4.2	0
172	Probing CAS database as prospective antiviral agents against SARS-CoV-2 main protease. *Journal of Molecular Structure*, **2021**, 1231, 129953	3.4	3
171	Mechanistic insights into the inhibitory activity of FDA approved ivermectin against SARS-CoV-2: old drug with new implications. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-12	3.6	1
170	Dithiocarbamate derivatives inhibit -glucosidase through an apparent allosteric site on the enzyme. *Chemical Biology and Drug Design*, **2021**, 98, 283-294	2.9	1
169	Exploiting Dengue Virus Protease as a Therapeutic Target: Current Status, Challenges and Future Avenues. *Current Medicinal Chemistry*, **2021**, 28, 7767-7802	4.3	1
168	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

167	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
166	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
165	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
164	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
163	Synthesis of azachalcones, their □amylase, □glucosidase inhibitory activities, kinetics, and molecular docking studies. *Bioorganic Chemistry*, **2021**, 106, 104489	5.1	16
162	Protonation states at different pH, conformational changes and impact of glycosylation in synapsin Ia. *Physical Chemistry Chemical Physics*, **2021**, 23, 16718-16729	3.6	0
161	Synthesis of Highly Potent Anti-Inflammatory Compounds (ROS Inhibitors) from Isonicotinic Acid. *Molecules*, **2021**, 26,	4.8	3
160	Structure and ligand-based drug discovery of IL-4 inhibitors via interaction-energy-based learning approaches. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-19	3.6	
159	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
158	Nicotinamide-cinnamic acid cocktail exerts pancreatic □cells survival coupled with insulin secretion through ERK1/2 signaling pathway in an animal model of apoptosis. *DARU, Journal of Pharmaceutical Sciences*, **2021**, 29, 483-492	3.9	
157	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
156	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
155	Phenylpyrazalopyrimidines as Tyrosine Kinase Inhibitors: Synthesis, Antiproliferative Activity, and Molecular Simulations. *Molecules*, **2020**, 25,	4.8	6
154	Enamine Barbiturates and Thiobarbiturates as a New Class of Bacterial Urease Inhibitors. *Applied Sciences (Switzerland)*, **2020**, 10, 3523	2.6	0
153	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
152	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
151	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
150	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

149	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
148	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
147	Molecular Docking Studies and Anti-Alzheimer Potential of Isolated Compounds from Tinospora cordifolia. *Journal of Biologically Active Products From Nature*, **2020**, 10, 100-121	0.7	1
146	2-Mercapto Benzothiazole Derivatives: As Potential Leads for the Diabetic Management. *Medicinal Chemistry*, **2020**, 16, 826-840	1.8	4
145	Synthesis of Novel 8-Hydroxyquinoline Derivatives through Mannich Reaction and their Biological Evaluation as Potential Immunomodulatory Agents. *Medicinal Chemistry*, **2020**, 16, 531-543	1.8	1
144	Computational Overview of Mycobacterial Thymidine Monophosphate Kinase. *Current Pharmaceutical Design*, **2020**, 26, 1676-1681	3.3	0
143	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
142	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
141	Structure, Antimicrobial Activity, Hirshfeld Analysis, and Docking Studies of Three Silver(I) Complexes-Based Pyridine Ligands. *Applied Sciences (Switzerland)*, **2020**, 10, 4853	2.6	1
140	4-Benzyloxylonchocarpin and Muracatanes A-C from L. and Their Biological Effects. *Biomolecules*, **2020**, 10,	5.9	1
139	Synthetic flavonoids as potential antiviral agents against SARS-CoV-2 main protease. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-12	3.6	12
138	Identification of novel Epac2 antagonists through in silico and in vitro analyses. *European Journal of Pharmaceutical Sciences*, **2020**, 153, 105492	5.1	0
137	Anti-urease and cytotoxic activity of 1-Nitro-2-phenylethane and Nerolidol; two major compounds isolated from the seeds of Dennettia tripetala. *Medicinal Chemistry Research*, **2020**, 29, 1874-1881	2.2	1
136	Quantum mechanics and 3D-QSAR studies on thienopyridine analogues: inhibitors of IKK *Heliyon*, **2020**, 6, e04125	3.6	3
135	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
134	Synthesis of a New Class of Spirooxindole-Benzo Thiophene-Based Molecules as Acetylcholinesterase Inhibitors. *Molecules*, **2020**, 25,	4.8	8
133	Novel 4,6-Disubstituted -Triazin-2-yl Amino Acid Derivatives as Promising Antifungal Agents. *Journal of Fungi (Basel, Switzerland)*, **2020**, 6,	5.6	4
132	Discovery of Potential Chemical Probe as Inhibitors of CXCL12 Using Ligand-Based Virtual Screening and Molecular Dynamic Simulation. *Molecules*, **2020**, 25,	4.8	3

131	Identification of potential TNF- inhibitors: from in silico to in vitro studies. *Scientific Reports*, **2020**, 10, 20974	4.9	8
130	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
129	Synthesis of Oxindole Analogues, Biological Activity, and In Silico Studies. *ChemistrySelect*, **2019**, 4, 10510-10516	1.8	9
128	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
127	Deciphering the Role of PKC in Calpain-CAST System Through Formal Modeling Approach. *Lecture Notes in Computer Science*, **2019**, 60-71	0.9	1
126	Coumarin derivatives as acetyl- and butyrylcholinestrase inhibitors: An in vitro, molecular docking, and molecular dynamics simulations study. *Heliyon*, **2019**, 5, e01552	3.6	13
125	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
124	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
123	Purification and Characterization of a Nonspecific Lipid Transfer Protein 1 (nsLTP1) from Ajwain (Trachyspermum ammi) Seeds. *Scientific Reports*, **2019**, 9, 4148	4.9	9
122	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
121	Exploring Novel -Myristoyltransferase Inhibitors: A Molecular Dynamics Simulation Approach. *ACS Omega*, **2019**, 4, 13658-13670	3.9	4
120	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
119	Inhibitory Effects of Myrtucommuacetalone 1 (MCA-1) from on Inflammatory Response in Mouse Macrophages. *Molecules*, **2019**, 25,	4.8	1
118	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
117	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
116	Insulin releasing effect of some pure compounds from Moringa oleifera on mice islets. *Medicinal Chemistry Research*, **2018**, 27, 1408-1418	2.2	8
115	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
114	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

113	Computational and biological characterization of fusion proteins of two insecticidal proteins for control of insect pests. *Scientific Reports*, **2018**, 8, 4837	4.9	5
112	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
111	Analyzing the Behavior of Neuronal Pathways in Alzheimer's Disease Using Petri Net Modeling Approach. *Frontiers in Neuroinformatics*, **2018**, 12, 26	3.9	9
110	Characterization of the interactions between coumarin-derivatives and acetylcholinesterase: Examination by NMR and docking simulations. *Journal of Molecular Modeling*, **2018**, 24, 207	2	7
109	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
108	Protein kinase A-dependent insulinotropic effect of selected flavonoids. *International Journal of Biological Macromolecules*, **2018**, 119, 149-156	7.9	2
107	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
106	Synthesis, antimicrobial activity, pharmacophore modeling and molecular docking studies of new pyrazole-dimedone hybrid architectures. *Chemistry Central Journal*, **2018**, 12, 29		19
105	2-Oxo-1,2,3,4-tetrahydropyrimidines Ethyl Esters as Potent □Glucuronidase Inhibitors: One-pot Synthesis, In vitro and In silico Studies. *Medicinal Chemistry*, **2018**, 14, 818-830	1.8	1
104	Eriodictyol stimulates insulin secretion through cAMP/PKA signaling pathway in mice islets. *European Journal of Pharmacology*, **2018**, 820, 245-255	5.3	25
103	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
102	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
101	Molecular dynamics simulation of interleukin-2 and its complex and determination of the binding free energy. *Molecular Simulation*, **2018**, 44, 1411-1425	2	4
100	Catalytic asymmetric synthesis of indole derivatives as novel □glucosidase inhibitors in vitro. *Bioorganic Chemistry*, **2018**, 79, 350-354	5.1	20
99	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
98	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
97	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
96	Synthesis of thiobarbituric acid derivatives: In vitro □glucosidase inhibition and molecular docking studies. *Bioorganic Chemistry*, **2017**, 75, 99-105	5.1	19

95	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
94	□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
93	Superoxide Scavenging and Antiglycation Activity of Rhinacanthins-rich Extract Obtained from the Leaves of. *Pharmacognosy Magazine*, **2017**, 13, 652-658	0.8	12
92	Synthesis of pyrimidine-2,4,6-trione derivatives: Anti-oxidant, anti-cancer, □glucosidase, □glucuronidase inhibition and their molecular docking studies. *Bioorganic Chemistry*, **2016**, 68, 72-9	5.1	35
91	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
90	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
89	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
88	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
87	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
86	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
85	In-silico identification of the binding mode of synthesized adamantyl derivatives inside cholinesterase enzymes. *Acta Pharmacologica Sinica*, **2015**, 36, 879-86	8	11
84	BRAF gene: From human cancers to developmental syndromes. *Saudi Journal of Biological Sciences*, **2015**, 22, 359-73	4	44
83	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
82	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
81	Synthesis and dynamics studies of barbituric acid derivatives as urease inhibitors. *Chemistry Central Journal*, **2015**, 9, 63		19
80	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
79	Gd-Complexes of New Arylpiperazinyl Conjugates of DTPA-Bis(amides): Synthesis, Characterization and Magnetic Relaxation Properties. *Molecules*, **2015**, 20, 7807-19	4.8	1
78	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

77	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
76	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
75	Molecular docking- and genetic algorithm-based approaches to produce robust 3D-QSAR models. *Medicinal Chemistry Research*, **2014**, 23, 2198-2206	2.2	1
74	CoMFA and CoMSIA studies on a series of fluroquinolone derivatives for potential anti-inflammatory activity. *Analytical Methods*, **2014**, 6, 6823	3.2	1
73	Structure-based 3D-QSAR studies on quinazoline derivatives as platelets-derived growth factor (PDGFR) inhibitors. *Medicinal Chemistry Research*, **2014**, 23, 4070-4084	2.2	
72	Structure-based design, synthesis and biological evaluation of β-glucuronidase inhibitors. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 577-85	4.2	30
71	Synthesis, anti-microbial and molecular docking studies of quinazolin-4(3H)-one derivatives. *Molecules*, **2014**, 19, 8725-39	4.8	14
70	Structural basis of binding and rationale for the potent urease inhibitory activity of biscoumarins. *BioMed Research International*, **2014**, 2014, 935039	3	9
69	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
68	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
67	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
66	Design of new and potent diethyl thiobarbiturates as urease inhibitors: a computational approach. *Bioinformation*, **2014**, 10, 299-307	1.1	
65	Identification of novel Interleukin-2 inhibitors through computational approaches. *Molecular Diversity*, **2013**, 17, 345-55	3.1	17
64	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
63	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
62	Molecular docking simulation studies on potent butyrylcholinesterase inhibitors obtained from microbial transformation of dihydrotestosterone. *Chemistry Central Journal*, **2013**, 7, 164		7
61	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
60	Crude to leads: a triple-pronged direct NMR approach in coordination with docking simulation. *Analyst, The*, **2013**, 138, 5137-45	5	6

59	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
58	A combined 3D-QSAR and docking studies for the In-silico prediction of HIV-protease inhibitors. *Chemistry Central Journal*, **2013**, 7, 88		9
57	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
56	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
55	In silico identification of novel inhibitors against Plasmodium falciparum dihydroorate dehydrogenase. *Journal of Molecular Graphics and Modelling*, **2013**, 40, 40-7	2.8	15
54	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
53	In-silico analysis of chromone containing sulfonamide derivatives as human carbonic anhydrase inhibitors. *Medicinal Chemistry*, **2013**, 9, 608-16	1.8	3
52	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
51	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
50	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
49	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
48	Docking based 3D-QSAR studies applied at the BRAF inhibitors to understand the binding mechanism. *Journal of Cheminformatics*, **2012**, 4,	8.6	78
47	In silico studies on 2,3-dihydro-1,5-benzothiazepines as cholinesterase inhibitors. *Medicinal Chemistry Research*, **2012**, 21, 2329-2339	2.2	10
46	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
45	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
44	Molecular docking studies of potent inhibitors of tyrosinase and □glucosidase. *Medicinal Chemistry Research*, **2012**, 21, 1677-1683	2.2	19
43	Synthesis and QSAR analysis of chalcone derivatives as nitric oxide inhibitory agent. *Medicinal Chemistry Research*, **2012**, 21, 1953-1966	2.2	12
42	In silico and in vitro immunomodulatory studies on compounds of Lindelofia stylosa. *Chemical Biology and Drug Design*, **2012**, 79, 290-9	2.9	24

41	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
40	Molecular modeling-based antioxidant arylidene barbiturates as urease inhibitors. *Journal of Molecular Graphics and Modelling*, **2011**, 30, 153-6	2.8	34
39	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
38	Docking and 3D-QSAR modeling of cyclin-dependent kinase 5/p25 inhibitors. *Journal of Molecular Modeling*, **2011**, 17, 1149-61	2	9
37	Molecular dynamics simulation of mammalian 15S-lipoxygenase with AMBER force field. *European Biophysics Journal*, **2011**, 40, 715-26	1.9	14
36	Optimization of Structure Based Virtual Screening Protocols Against Thymidine Monophosphate Kinase Inhibitors as Antitubercular Agents. *Molecular Informatics*, **2011**, 30, 851-62	3.8	5
35	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
34	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
33	Immunosuppressive activity of buxidin and E-buxenone from Buxus hyrcana. *Chemical Biology and Drug Design*, **2010**, 75, 310-7	2.9	23
32	Identification of novel urease inhibitors by high-throughput virtual and in vitro screening. *ACS Medicinal Chemistry Letters*, **2010**, 1, 145-9	4.3	58
31	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
30	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
29	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
28	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
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