Mohammad Shahidul Islam

List of Publications by Year
in descending order

188 papers	2,755 citations	218592 26 h-index	302012 39 g-index
192 all docs	192 docs citations	192 times ranked	3581 citing authors

#	Article	IF	Citations
1	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
2	Synthesis of new thiazolo-pyrrolidineâ€“(spirooxindole) tethered to 3-acylindole as anticancer agents. Bioorganic Chemistry, 2019, 82, 423-430.	2.0	66
3	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
4	Substituted spirooxindole derivatives as potent anticancer agents through inhibition of phosphodiesterase 1. RSC Advances, 2018, 8, 14335-14346.	1.7	57
5	Design and synthesis of new substituted spirooxindoles as potential inhibitors of the MDM2â€“p53 interaction. Bioorganic Chemistry, 2019, 86, 598-608.	2.0	52
6	Heavy Metal Ions Removal from Aqueous Solutions by Treated Ajwa Date Pits: Kinetic, Isotherm, and Thermodynamic Approach. Polymers, 2022, 14, 914.	2.0	51
7	Highly enantioselective Friedelâ€“Crafts alkylation of indoles with Î±,Î²-unsaturated ketones with simple Cu(II)â€“oxazolineâ€“imidazoline catalysts. Tetrahedron, 2013, 69, 5185-5192.	1.0	49
8	Catalytic asymmetric synthesis of indole derivatives as novel Î±-glucosidase inhibitors in vitro. Bioorganic Chemistry, 2018, 79, 350-354.	2.0	44
9	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
10	Synthesis, in vitro biological activities and in silico study of dihydropyrimidines derivatives. Bioorganic and Medicinal Chemistry, 2015, 23, 6740-6748.	1.4	42
11	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
12	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
13	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
14	Identification of potential TNF-Î± inhibitors: from in silico to in vitro studies. Scientific Reports, 2020, 10, 20974.	1.6	39
15	Synthesis of azachalcones, their Î±-amylase, Î±-glucosidase inhibitory activities, kinetics, and molecular docking studies. Bioorganic Chemistry, 2021, 106, 104489.	2.0	39
16	Highly enantioselective Friedelâ€“Crafts alkylation of indole with electron deficient trans-Î²-nitroalkenes using Zn(II)â€“oxazolineâ€“imidazoline catalysts. Tetrahedron: Asymmetry, 2014, 25, 245-251.	1.8	38
17	New spiro-oxindole constructed with pyrrolidine/thioxothiazolidin-4-one derivatives: Regioselective synthesis, X-ray crystal structures, Hirshfeld surface analysis, DFT, docking and antimicrobial studies. Journal of Molecular Structure, 2018, 1152, 101-114.	1.8	37
18	Eriodictyol stimulates insulin secretion through cAMP/PKA signaling pathway in mice islets. European Journal of Pharmacology, 2018, 820, 245-255.	1.7	37

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19	Synthesis and characterization of 2-substituted benzimidazoles and their evaluation as anticancer agent. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 142, 286-291.	2.0	36
20	Towards environmentally friendlier Suzukiâ€“Miyaura reactions with precursors of Pd-NHC (NHC =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	4.6	36
21	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
22	Synthesis, Structural Characterization and Antimicrobial Activity of Cu(II) and Fe(III) Complexes Incorporating Azo-Azomethine Ligand. Molecules, 2018, 23, 813.	1.7	31
23	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
24	Cu(II) salen complex with propylene linkage: An efficient catalyst in the formation of C X bonds (XÂ=ÂN,) Tj ETQq0 0 0 rgBT /Overlock 10	1.8	30
25	Fluorescein hydrazones: A series of novel non-intercalative topoisomerase IIÎ± catalytic inhibitors induce G1 arrest and apoptosis in breast and colon cancer cells. European Journal of Medicinal Chemistry, 2017, 125, 49-67.	2.6	30
26	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
27	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
28	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
29	Synthesis, antimicrobial activity, pharmacophore modeling and molecular docking studies of new pyrazole-dimedone hybrid architectures. Chemistry Central Journal, 2018, 12, 29.	2.6	28
30	Coumarin derivatives as acetyl- and butyrylcholinestrase inhibitors: An inÂvitro, molecular docking, and molecular dynamics simulations study. Heliyon, 2019, 5, e01552.	1.4	28
31	Facile synthesis of Pd@graphene nanocomposites with enhanced catalytic activity towards Suzuki coupling reaction. Scientific Reports, 2020, 10, 11728.	1.6	26
32	Synthesis of thiobarbituric acid derivatives: In vitro Î± -glucosidase inhibition and molecular docking studies. Bioorganic Chemistry, 2017, 75, 99-105.	2.0	25
33	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
34	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
35	Synthesis, Anticancer Activity, and Molecular Modeling of New Halogenated Spiro[pyrrolidine-thiazolo-oxindoles] Derivatives. Applied Sciences (Switzerland), 2020, 10, 2170.	1.3	24
36	Synthesis and dynamics studies of barbituric acid derivatives as urease inhibitors. Chemistry Central Journal, 2015, 9, 63.	2.6	23

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37	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
38	Palladate Precatalysts for the Formation of Câ€“N and Câ€“C Bonds. Organometallics, 2019, 38, 2812-2817.	1.1	23
39	Regio- and Stereoselective Synthesis of a New Series of Spirooxindole Pyrrolidine Grafted Thiochromene Scaffolds as Potential Anticancer Agents. Symmetry, 2021, 13, 1426.	1.1	23
40	Purification and Characterization of a Nonspecific Lipid Transfer Protein 1 (nsLTP1) from Ajwain (Trachyspermum ammi) Seeds. Scientific Reports, 2019, 9, 4148.	1.6	21
41	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
42	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
43	Synthesis, Anti-microbial and Molecular Docking Studies of Quinazolin-4(3H)-one Derivatives. Molecules, 2014, 19, 8725-8739.	1.7	19
44	Synthesis of novel 5-monoalkylbarbiturate derivatives: new access to 1,2-oxazepines. Tetrahedron Letters, 2015, 56, 6984-6987.	0.7	19
45	Tandem Knoevenagelâ€“Michael reactions in aqueous diethylamine medium: A greener and efficient approach toward bis-dimedone derivatives. Arabian Journal of Chemistry, 2017, 10, 185-193.	2.3	19
46	Superoxide scavenging and antiglycation activity of rhinacanthins-rich extract obtained from the leaves of Rhinacanthus nasutus. Pharmacognosy Magazine, 2017, 13, 652.	0.3	19
47	A concise synthesis and evaluation of new malonamide derivatives as potential Î±-glucosidase inhibitors. Bioorganic and Medicinal Chemistry, 2016, 24, 1675-1682.	1.4	18
48	Construction of Spirooxindole Analogues Engrafted with Indole and Pyrazole Scaffolds as Acetylcholinesterase Inhibitors. ACS Omega, 2021, 6, 31539-31556.	1.6	18
49	Ligandâ€based 3Dâ€QSAR Studies of Physostigmine Analogues as Acetylcholinesterase Inhibitors. Chemical Biology and Drug Design, 2009, 74, 571-581.	1.5	17
50	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
51	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
52	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
53	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
54	2-Mercapto Benzothiazole Derivatives: As Potential Leads for the Diabetic Management. Medicinal Chemistry, 2020, 16, 826-840.	0.7	17

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55	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
56	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
57	Synthesis of Oxindole Analogues, Biological Activity, and In Silico Studies. ChemistrySelect, 2019, 4, 10510-10516.	0.7	16
58	Synthesis of a New Class of Spirooxindoleâ€“Benzo[b]Thiophene-Based Molecules as Acetylcholinesterase Inhibitors. Molecules, 2020, 25, 4671.	1.7	16
59	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
60	Removal of Chromium(III) and Cadmium(II) Heavy Metal Ions from Aqueous Solutions Using Treated Date Seeds: An Eco-Friendly Method. Molecules, 2021, 26, 3718.	1.7	15
61	Structural Basis of Binding and Rationale for the Potent Urease Inhibitory Activity of Biscoumarins. BioMed Research International, 2014, 2014, 1-12.	0.9	14
62	Stereoselective synthesis of diazaspiro[5.5]undecane derivatives via base promoted [5+1] double Michael addition of N,N-dimethylbarbituric acid to diaryliedene acetones. Arabian Journal of Chemistry, 2017, 10, 1-9.	2.3	14
63	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
64	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
65	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
66	Isatin thiazoles as antidiabetic: Synthesis, in vitro enzyme inhibitory activities, kinetics, and in silico studies. Archiv Der Pharmazie, 2022, 355, e2100481.	2.1	14
67	Synthesis and Antiproliferative Activity of a New Series of Mono- and Bis(dimethylpyrazolyl)-s-triazine Derivatives Targeting EGFR/PI3K/AKT/mTOR Signaling Cascades. ACS Omega, 2022, 7, 24858-24870.	1.6	14
68	Synthesis and QSAR analysis of chalcone derivatives as nitric oxide inhibitory agent. Medicinal Chemistry Research, 2012, 21, 1953-1966.	1.1	13
69	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
70	Synthesis and Inhibitory Effect of Some Indoleâ€Pyrimidine Based Hybrid Heterocycles on Î±â€Glucosidase and Î±â€Amylase as Potential Hypoglycemic Agents. ChemistryOpen, 2019, 8, 1288-1297.	0.9	13
71	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
72	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

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73	Stereoselective Synthesis of the Di-Spirooxindole Analogs Based Oxindole and Cyclohexanone Moieties as Potential Anticancer Agents. Molecules, 2021, 26, 6305.	1.7	13
74	In-silico identification of the binding mode of synthesized adamantyl derivatives inside cholinesterase enzymes. Acta Pharmacologica Sinica, 2015, 36, 879-886.	2.8	12
75	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
76	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
77	Quantum chemical insight into the molecular structure of L-chemosensor 1,3-dimethyl-5-(thien-2-ylmethylene)-pyrimidine-2,4,6-(1H,3H,5H)-trione: Naked-eye colorimetric detection of copper(II) anions. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850005.	1.8	12
78	Analyzing the Behavior of Neuronal Pathways in Alzheimer's Disease Using Petri Net Modeling Approach. Frontiers in Neuroinformatics, 2018, 12, 26.	1.3	12
79	Anticancer Indole-Based Chalcones: A Structural and Theoretical Analysis. Molecules, 2019, 24, 3728.	1.7	12
80	Synthesis of Pyridine-Dicarboxamide-Cyclohexanone Derivatives: Anticancer and Î±-Glucosidase Inhibitory Activities and In Silico Study. Molecules, 2019, 24, 1332.	1.7	12
81	Synthesis, structural investigations and pharmacological properties of a new zinc complex with a N4-donor Schiff base incorporating 2-pyridyl ring. Inorganica Chimica Acta, 2019, 487, 97-106.	1.2	12
82	Design, Construction, and Characterization of a New Regioisomer and Diastereomer Material Based on the Spirooxindole Scaffold Incorporating a Sulphone Function. Symmetry, 2020, 12, 1337.	1.1	12
83	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
84	A combined 3D-QSAR and docking studies for the In-silicoprediction of HIV-protease inhibitors. Chemistry Central Journal, 2013, 7, 88.	2.6	11
85	Exploring Novel N-Myristoyltransferase Inhibitors: A Molecular Dynamics Simulation Approach. ACS Omega, 2019, 4, 13658-13670.	1.6	11
86	Mizorokiâ€“Heck Crossâ€Coupling of Acrylate Derivatives with Aryl Halides Catalyzed by Palladate Preâ€Catalysts. European Journal of Inorganic Chemistry, 2019, 2019, 4695-4699.	1.0	11
87	Synthesis of spiroindolone analogue via three components reaction of olefin with isatin and sarcosine: Anti-proliferative activity and computational studies. Journal of Molecular Structure, 2020, 1204, 127500.	1.8	11
88	Synthesis, X-ray Single Crystal, Conformational Analysis and Cholinesterase Inhibitory Activity of a New Spiropyrrolidine Scaffold Tethered Benzo[b]Thiophene Analogue. Crystals, 2020, 10, 120.	1.0	11
89	Regio- and stereoselective synthesis of spiro-heterocycles bearing the pyrazole scaffold via [3+2] cycloaddition reaction. Journal of Molecular Structure, 2022, 1250, 131711.	1.8	11
90	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

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91	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
92	Insulin releasing effect of some pure compounds from Moringa oleifera on mice islets. Medicinal Chemistry Research, 2018, 27, 1408-1418.	1.1	10
93	Computational and biological characterization of fusion proteins of two insecticidal proteins for control of insect pests. Scientific Reports, 2018, 8, 4837.	1.6	10
94	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
95	Inhibitory Effects of Myrtucommuacetalone 1 (MCA-1) from Myrtus Communis on Inflammatory Response in Mouse Macrophages. Molecules, 2020, 25, 13.	1.7	10
96	Phenylpyrazalopyrimidines as Tyrosine Kinase Inhibitors: Synthesis, Antiproliferative Activity, and Molecular Simulations. Molecules, 2020, 25, 2135.	1.7	10
97	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
98	Dinuclear uranium(vi) salen coordination compound: an efficient visible-light-active catalyst for selective reduction of CO2 to methanol. Dalton Transactions, 2020, 49, 17243-17251.	1.6	9
99	Synthesis of Spirooxindole Analogs Tethered Pyrazole Scaffold as Acetylcholinesterase Inhibitors. ChemistrySelect, 2021, 6, 14039-14053.	0.7	9
100	Synthesis, Molecular Structure and Spectroscopic Investigations of Novel Fluorinated Spiro Heterocycles. Molecules, 2015, 20, 8223-8241.	1.7	8
101	4-Benzyloxylonchocarpin and Muracatanes A-C from Ranunculus muricatus L. and Their Biological Effects. Biomolecules, 2020, 10, 1562.	1.8	8
102	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
103	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
104	Probing CAS database as prospective antiviral agents against SARS-CoV-2 main protease. Journal of Molecular Structure, 2021, 1231, 129953.	1.8	8
105	Facile Synthesis and Characterization of Palladium@Carbon Catalyst for the Suzuki-Miyaura and Mizoroki-Heck Coupling Reactions. Applied Sciences (Switzerland), 2021, 11, 4822.	1.3	8
106	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
107	Synthesis, Crystal Structure and DFT Studies of a New Dinuclear Ag(I)-Malonamide Complex. Molecules, 2018, 23, 888.	1.7	7
108	Protein kinase A-dependent insulinotropic effect of selected flavonoids. International Journal of Biological Macromolecules, 2018, 119, 149-156.	3.6	7

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109	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
110	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
111	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
112	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
113	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
114	Asymmetric Henry Reaction of Nitromethane with Substituted Aldehydes Catalyzed by Novel In Situ		

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127	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
128	Synthesis, computational studies and biological activity of oxamohydrazide derivatives bearing isatin and ferrocene scaffolds. Journal of Molecular Structure, 2020, 1202, 127372.	1.8	5
129	Quantum mechanics and 3D-QSAR studies on thienopyridine analogues: inhibitors of IKKÎ². Heliyon, 2020, 6, e04125.	1.4	5
130	Enamine Barbiturates and Thiobarbiturates as a New Class of Bacterial Urease Inhibitors. Applied Sciences (Switzerland), 2020, 10, 3523.	1.3	5
131	Synthesis, characterization of Uranyl(VI), Th(IV), Zr(IV) mixed-ligand complexes with S-methyl-2-(4-methoxybenzylidine)dithiocarbazate and N-donor co-ligand, and their evaluation as antimicrobial agent. Journal of Saudi Chemical Society, 2021, 25, 101207.	2.4	5
132	Bimetallic Ironâ€“Palladium Catalyst System as a Lewis-Acid for the Synthesis of Novel Pharmacophores Based Indole Scaffold as Anticancer Agents. Molecules, 2021, 26, 2212.	1.7	5
133	Exploiting the Chiral Ligands of Bis(imidazolinyl)- and Bis(oxazolinyl)thiophenesâ€”Synthesis and Application in Cu-Catalyzed Friedelâ€“Crafts Asymmetric Alkylation. Molecules, 2021, 26, 7408.	1.7	5
134	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
135	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
136	Facile and Promising Method for Michael Addition of Indole and Pyrrole to Electron-Deficienttrans-Î²-Nitroolefins Catalyzed by a Hydrogen Bond Donor Catalyst Feistâ€™s Acid and Preliminary Study of Antimicrobial Activity. Scientific World Journal, The, 2014, 2014, 1-15.	0.8	4
137	Molecular structure investigation and tautomerism aspects of (E)-3-benzylideneindolin-2-one. Journal of Chemical Sciences, 2015, 127, 1547-1556.	0.7	4
138	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
139	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
140	Exploiting Dengue Virus Protease as a Therapeutic Target: Current Status, Challenges and Future Avenues. Current Medicinal Chemistry, 2021, 28, 7767-7802.	1.2	4
141	In-Silico Analysis of Chromone Containing Sulfonamide Derivatives as Human Carbonic Anhydrase Inhibitors. Medicinal Chemistry, 2013, 9, 608-616.	0.7	4
142	Computational Overview of Mycobacterial Thymidine Monophosphate Kinase. Current Pharmaceutical Design, 2020, 26, 1676-1681.	0.9	4
143	Molecular Docking Studies and Anti-Alzheimerâ€™s Potential of Isolated Compounds fromTinospora cordifolia. Journal of Biologically Active Products From Nature, 2020, 10, 100-121.	0.1	4
144	Cu(<scp>ii</scp>)-thiophene-2,5-bis(amino-alcohol) mediated asymmetric Aldol reaction and Domino Knoevenagel Michael cyclization: a new highly efficient Lewis acid catalyst. RSC Advances, 2022, 12, 6149-6165.	1.7	4

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145	Sarcorucinine-D Inhibits Cholinesterases and Calcium Channels: Molecular Dynamics Simulation and In Vitro Mechanistic Investigations. Molecules, 2022, 27, 3361.	1.7	4
146	Synthesis of Some C₂â€Symmetric Bidentate Ligands and Their Complexes Derived from Feist's Acid. Helvetica Chimica Acta, 2012, 95, 268-277.	1.0	3
147	Molecular docking- and genetic algorithm-based approaches to produce robust 3D-QSAR models. Medicinal Chemistry Research, 2014, 23, 2198-2206.	1.1	3
148	5-[(3-Fluorophenyl)(2-hydroxy-6-oxocyclohex-1-en-1-yl)methyl]-6-hydroxy-1,3-dimethylpyrimidine-2,4(1H,3H)-dione. MolBank, 2016, 2016, M910.	0.2	3
149	Structure, Antimicrobial Activity, Hirshfeld Analysis, and Docking Studies of Three Silver(I) Complexes-Based Pyridine Ligands. Applied Sciences (Switzerland), 2020, 10, 4853.	1.3	3
150	X-ray Crystal Structure and Hirshfeld Analysis of Gem-Aminals-Based Morpholine, Pyrrolidine, and Piperidine Moieties. Symmetry, 2021, 13, 20.	1.1	3
151	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, 243-249.	0.3	3
152	Synthesis and anti-Cancer Activity of a New Hybrid Based Spirooxindole-Pyrrolidine -Thiochromene Scaffolds via [3â€‰+â€‰2] Cycloaddition Reaction: Computational Investigation. Polycyclic Aromatic Compounds, 2023, 43, 2302-2320.	1.4	3
153	Molecular dynamics simulation of Axillaridineâ€“A: A potent natural cholinesterase inhibitor. Journal of Enzyme Inhibition and Medicinal Chemistry, 2009, 24, 1101-1105.	2.5	2
154	Ligandâ€Based 3Dâ€QSAR Studies of Diaryl Acylâ€sulfonamide Analogues as Human Umbilical Vein Endothelial Cells Inhibitors Stimulated by VEGF. Chemical Biology and Drug Design, 2011, 77, 288-294.	1.5	2
155	Gd-Complexes of New Arylpiperazinyl Conjugates of DTPA-Bis(amides): Synthesis, Characterization and Magnetic Relaxation Properties. Molecules, 2015, 20, 7807-7819.	1.7	2
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