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	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
2	Syntheses, in vitro, and in silico studies of rhodanine-based schiff bases as potential Î±-amylase inhibitors and radicals (DPPH and ABTS) scavengers. Molecular Diversity, 2023, 27, 767-791.	2.1	2
3	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
4	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, 2022, 40, 4399-4408.	2.0	2
5	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
6	Theoretical investigation of selective ligand binding mode of galanin receptors. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12964-12974.	2.0	2
7	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
8	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
9	Effects of Smokeless Tobacco Samples from Tabuk Saudi Arabia on Nitric Oxide Production: A Potential Risk for Cancer and Cardiovascular Diseases. Current Computer-Aided Drug Design, 2022, 18, 110-119.	0.8	1
10	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
11	Heavy Metal Ions Removal from Aqueous Solutions by Treated Ajwa Date Pits: Kinetic, Isotherm, and Thermodynamic Approach. Polymers, 2022, 14, 914.	2.0	51
12	Isatin thiazoles as antidiabetic: Synthesis, in vitro enzyme inhibitory activities, kinetics, and in silico studies. Archiv Der Pharmazie, 2022, 355, e2100481.	2.1	14
13	Structure-Based Virtual Screening to Identify Negative Allosteric Modulators of NMDA. Medicinal Chemistry, 2022, 18, .	0.7	2
14	Pyrene Functionalized Highly Reduced Graphene Oxide-palladium Nanocomposite: A Novel Catalyst for the Mizoroki-Heck Reaction in Water. Frontiers in Chemistry, 2022, 10, 872366.	1.8	2
15	Mechanistic Evaluation of the Stability of Arylvinyl-1,2,4-trioxanes under Acidic Conditions for Their Oral Administration as an Antimalarial Drug. ACS Omega, 2022, 7, 17984-17994.	1.6	1
16	Sarcorucinine-D Inhibits Cholinesterases and Calcium Channels: Molecular Dynamics Simulation and In Vitro Mechanistic Investigations. Molecules, 2022, 27, 3361.	1.7	4
17	Antibacteria, Antiurease, and Antiproliferative Abruquinones from Abrus precatorius Roots. Journal of Biologically Active Products From Nature, 2022, 12, 276-290.	0.1	0
18	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

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19	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
20	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
21	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
22	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
23	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
24	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
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	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.	2.0	0
27	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
28	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.	2.0	2
29	Exploring the Molecular Mechanisms of 17Î²-HSD5-induced Carcinogenicity of Catha edulis via Molecular Modeling Approach. Medicinal Chemistry, 2021, 17, 418-428.	0.7	0
30	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
31	Site-directed Fragnomics and MD Simulations Approaches to Identify Interleukin-2 Inhibitors. Medicinal Chemistry, 2021, 17, 407-417.	0.7	0
32	Characterization of the multidrug efflux transporter <scp>styMdtM</scp> from <scp>Salmonella enterica</scp> serovar Typhi. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1193-1204.	1.5	2
33	Probing CAS database as prospective antiviral agents against SARS-CoV-2 main protease. Journal of Molecular Structure, 2021, 1231, 129953.	1.8	8
34	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
35	Synthesis and X-ray crystal structure of unexpected novel thiazolidinone/1,3,4-thiadiazole heterocycle via S-alkylation and Smiles rearrangement dual approaches. Journal of Molecular Structure, 2021, 1234, 130156.	1.8	2
36	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

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37	Exploiting Dengue Virus Protease as a Therapeutic Target: Current Status, Challenges and Future Avenues. Current Medicinal Chemistry, 2021, 28, 7767-7802.	1.2	4
38	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
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	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
41	Asymmetric Henry Reaction of Nitromethane with Substituted Aldehydes Catalyzed by Novel In Situ		

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55	4-Benzyloxylonchocarpin and Muracatanes A-C from Ranunculus muricatus L. and Their Biological Effects. Biomolecules, 2020, 10, 1562.	1.8	8
56	Identification of novel Epac2 antagonists through in silico and in vitro analyses. European Journal of Pharmaceutical Sciences, 2020, 153, 105492.	1.9	2
57	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.	1.1	1
58	Quantum mechanics and 3D-QSAR studies on thienopyridine analogues: inhibitors of IKKÎ². Heliyon, 2020, 6, e04125.	1.4	5
59	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
60	Synthesis of a New Class of Spirooxindoleâ€“Benzo[b]Thiophene-Based Molecules as Acetylcholinesterase Inhibitors. Molecules, 2020, 25, 4671.	1.7	16
61	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
62	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
63	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
64	Identification of potential TNF-Î± inhibitors: from in silico to in vitro studies. Scientific Reports, 2020, 10, 20974.	1.6	39
65	Phenylpyrazalopyrimidines as Tyrosine Kinase Inhibitors: Synthesis, Antiproliferative Activity, and Molecular Simulations. Molecules, 2020, 25, 2135.	1.7	10
66	Enamine Barbiturates and Thiobarbiturates as a New Class of Bacterial Urease Inhibitors. Applied Sciences (Switzerland), 2020, 10, 3523.	1.3	5
67	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
68	Synthesis, Anticancer Activity, and Molecular Modeling of New Halogenated Spiro[pyrrolidine-thiazolo-oxindoles] Derivatives. Applied Sciences (Switzerland), 2020, 10, 2170.	1.3	24
69	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
70	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
71	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
72	One-Pot Synthesis, X-ray Single Crystal and Molecular Insight of Enaminone-Based Î²-Morpholino-/N-Methylpiperazinyl-/Pyrrolidinylpropiophenone. Crystals, 2020, 10, 282.	1.0	1

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73	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
74	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
75	Synthesis of Novel 8-Hydroxyquinoline Derivatives through Mannich Reaction and their Biological Evaluation as Potential Immunomodulatory Agents. Medicinal Chemistry, 2020, 16, 531-543.	0.7	2
76	Computational Overview of Mycobacterial Thymidine Monophosphate Kinase. Current Pharmaceutical Design, 2020, 26, 1676-1681.	0.9	4
77	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
78	2-Mercapto Benzothiazole Derivatives: As Potential Leads for the Diabetic Management. Medicinal Chemistry, 2020, 16, 826-840.	0.7	17
79	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
80	Exploring Novel N-Myristoyltransferase Inhibitors: A Molecular Dynamics Simulation Approach. ACS Omega, 2019, 4, 13658-13670.	1.6	11
81	Palladate Precatalysts for the Formation of Câ€“N and Câ€“C Bonds. Organometallics, 2019, 38, 2812-2817.	1.1	23
82	Anticancer Indole-Based Chalcones: A Structural and Theoretical Analysis. Molecules, 2019, 24, 3728.	1.7	12
83	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
84	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
85	Synthesis of Oxindole Analogues, Biological Activity, and In Silico Studies. ChemistrySelect, 2019, 4, 10510-10516.	0.7	16
86	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
87	Design and synthesis of new substituted spirooxindoles as potential inhibitors of the MDM2â€“p53 interaction. Bioorganic Chemistry, 2019, 86, 598-608.	2.0	52
88	Synthesis of Pyridine-Dicarboxamide-Cyclohexanone Derivatives: Anticancer and Î±-Glucosidase Inhibitory Activities and In Silico Study. Molecules, 2019, 24, 1332.	1.7	12
89	Coumarin derivatives as acetyl- and butyrylcholinestrase inhibitors: An inÂvitro, molecular docking, and molecular dynamics simulations study. Heliyon, 2019, 5, e01552.	1.4	28
90	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

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91	Purification and Characterization of a Nonspecific Lipid Transfer Protein 1 (nsLTP1) from Ajwain (Trachyspermum ammi) Seeds. Scientific Reports, 2019, 9, 4148.	1.6	21
92	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
93	Synthesis of new thiazolo-pyrrolidineâ€“(spirooxindole) tethered to 3-acylindole as anticancer agents. Bioorganic Chemistry, 2019, 82, 423-430.	2.0	66
94	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
95	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
96	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
97	Insulin releasing effect of some pure compounds from Moringa oleifera on mice islets. Medicinal Chemistry Research, 2018, 27, 1408-1418.	1.1	10
98	Substituted spirooxindole derivatives as potent anticancer agents through inhibition of phosphodiesterase 1. RSC Advances, 2018, 8, 14335-14346.	1.7	57
99	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
100	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
101	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
102	Computational and biological characterization of fusion proteins of two insecticidal proteins for control of insect pests. Scientific Reports, 2018, 8, 4837.	1.6	10
103	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
104	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
105	Eriodictyol stimulates insulin secretion through cAMP/PKA signaling pathway in mice islets. European Journal of Pharmacology, 2018, 820, 245-255.	1.7	37
106	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
107	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
108	Chemical reactivity, molecular structure, spectroscopic and DFT computational studies of spiro-heterocycle incorporating furan ring. Materials Express, 2018, 8, 335-344.	0.2	1

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109	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
110	Towards environmentally friendlier Suzukiâ€“Miyaura reactions with precursors of Pd-NHC (NHC =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	4.6	36
111	Catalytic asymmetric synthesis of indole derivatives as novel Î±-glucosidase inhibitors in vitro. Bioorganic Chemistry, 2018, 79, 350-354.	2.0	44
112	Analyzing the Behavior of Neuronal Pathways in Alzheimer's Disease Using Petri Net Modeling Approach. Frontiers in Neuroinformatics, 2018, 12, 26.	1.3	12
113	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
114	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
115	Synthesis, Structural Characterization and Antimicrobial Activity of Cu(II) and Fe(III) Complexes Incorporating Azo-Azomethine Ligand. Molecules, 2018, 23, 813.	1.7	31
116	Synthesis, Crystal Structure and DFT Studies of a New Dinuclear Ag(I)-Malonamide Complex. Molecules, 2018, 23, 888.	1.7	7
117	Protein kinase A-dependent insulinotropic effect of selected flavonoids. International Journal of Biological Macromolecules, 2018, 119, 149-156.	3.6	7
118	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
119	Synthesis, antimicrobial activity, pharmacophore modeling and molecular docking studies of new pyrazole-dimedone hybrid architectures. Chemistry Central Journal, 2018, 12, 29.	2.6	28
120	2-Oxo-1,2,3,4-tetrahydropyrimidines Ethyl Esters as Potent Î²- Glucuronidase Inhibitors: One-pot Synthesis, In vitro and In silico Studies. Medicinal Chemistry, 2018, 14, 818-830.	0.7	2
121	Isolation of flavonoides from Artemisia macrocephala anticholinesterase activity: Isolation, characterization and its in vitro anticholinesterse activity supported by molecular docking. Pakistan Journal of Pharmaceutical Sciences, 2018, 31, 1347-1354.	0.2	2
122	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
123	Monoalkylated barbiturate derivatives: X-ray crystal structure, theoretical studies, and biological activities. Journal of Molecular Structure, 2017, 1141, 624-633.	1.8	5
124	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
125	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
126	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

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127	Synthesis of thiobarbituric acid derivatives: In vitro Î± -glucosidase inhibition and molecular docking studies. Bioorganic Chemistry, 2017, 75, 99-105.	2.0	25
128	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
129	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
130	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
131	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
132	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
133	Enantioselective additions of diethylzinc to aldehydes catalyzed by titanate(IV) complex with chiral bidentate bis-amide ligands based on cyclopropane backbone. Arabian Journal of Chemistry, 2017, 10, S964-S970.	2.3	2
134	Superoxide scavenging and antiglycation activity of rhinacanthins-rich extract obtained from the leaves of Rhinacanthus nasutus. Pharmacognosy Magazine, 2017, 13, 652.	0.3	19
135	Molecular Structure, Spectroscopic and DFT Computational Studies of Arylidene-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione. Crystals, 2016, 6, 110.	1.0	2
136	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
137	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
138	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
139	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
140	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
141	Crystal structure of 5-((4-bromophenyl)(2-hydroxy-6-oxocyclohex-1-en-1-yl)methyl)-6-hydroxy-1,3-dimethylpyrimidine-2,4(1H,3H)-dione, C₁₉H₁₉BrN₂O₅. Zeitschrift Fur Kristallographie - New Crystal Structures, 2016, 231, 843-845.	0.1	0
142	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
143	Crystal structure of diethylammonium 1,3-dimethyl-2,4,6-trioxohexahydropyrimidin-5-ide, C₁₀H₁₉N₃O₃. Zeitschrift Fur Kristallographie - New Crystal Structures, 2016, 231, 1063-1064.	0.1	1
144	In silico based investigation of dynamic variations in neprilysin (NEP and NEP2) proteins for extracting the point of specificity. Molecular BioSystems, 2016, 12, 1024-1036.	2.9	1

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145	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
146	Molecular structure investigation and biological evaluation of Michael adducts derived from dimedone. Research on Chemical Intermediates, 2016, 42, 4041-4053.	1.3	6
147	Palladium complexes bearing the dipyridyl ligand: synthesis, structural studies, and use in the Heck reaction. Research on Chemical Intermediates, 2016, 42, 379-389.	1.3	0
148	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
149	Gd-Complexes of New Arylpiperazinyl Conjugates of DTPA-Bis(amides): Synthesis, Characterization and Magnetic Relaxation Properties. Molecules, 2015, 20, 7807-7819.	1.7	2
150	Synthesis, Molecular Structure and Spectroscopic Investigations of Novel Fluorinated Spiro Heterocycles. Molecules, 2015, 20, 8223-8241.	1.7	8
151	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
152	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
153	Crystal Structure of 7,11-bis(2,4-dichlorophenyl)-2,4-dimethyl-2,4- diazaspiro[5.5]undecane -1,3,5,9-tetraone and its computational studies. Journal of Chemical Sciences, 2015, 127, 2039-2050.	0.7	2
154	Molecular structure investigation and tautomerism aspects of (E)-3-benzylideneindolin-2-one. Journal of Chemical Sciences, 2015, 127, 1547-1556.	0.7	4
155	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
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