Ashfaq Ur Rehman

List of Publications by Year in descending order

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ACHEAO LID REHMAN

#	Article	IF	CITATIONS
1	Isatin based Schiff bases as inhibitors of α-glucosidase: Synthesis, characterization, in vitro evaluation and molecular docking studies. Bioorganic Chemistry, 2015, 60, 42-48.	4.1	147
2	Triazinoindole analogs as potent inhibitors of α-glucosidase: Synthesis, biological evaluation and molecular docking studies. Bioorganic Chemistry, 2015, 58, 81-87.	4.1	126
3	Discovery of cryptic allosteric sites using reversed allosteric communication by a combined computational and experimental strategy. Chemical Science, 2021, 12, 464-476.	7.4	84
4	Synthesis of benzotriazoles derivatives and their dual potential as α-amylase and α-glucosidase inhibitors inÂvitro: Structure-activity relationship, molecular docking, and kinetic studies. European Journal of Medicinal Chemistry, 2019, 183, 111677.	5.5	78
5	Novel quinoline derivatives as potent in vitro α-glucosidase inhibitors: in silico studies and SAR predictions. MedChemComm, 2015, 6, 1826-1836.	3.4	58
6	Synthesis of new indazole based dual inhibitors of α-glucosidase and α-amylase enzymes, their in vitro, in silico and kinetics studies. Bioorganic Chemistry, 2020, 94, 103195.	4.1	51
7	Structural and free energy landscape of novel mutations in ribosomal protein S1 (rpsA) associated with pyrazinamide resistance. Scientific Reports, 2019, 9, 7482.	3.3	48
8	Synthesis, α-glucosidase inhibitory, cytotoxicity and docking studies of 2-aryl-7-methylbenzimidazoles. Bioorganic Chemistry, 2016, 65, 100-109.	4.1	47
9	Synthesis of quinoline derivatives as diabetic II inhibitors and molecular docking studies. Bioorganic and Medicinal Chemistry, 2019, 27, 4081-4088.	3.0	45
10	Synthesis, in vitro urease inhibitory potential and molecular docking study of Benzimidazole analogues. Bioorganic Chemistry, 2019, 89, 103024.	4.1	45
11	Syntheses, in vitro α-amylase and α-glucosidase dual inhibitory activities of 4-amino-1,2,4-triazole derivatives their molecular docking and kinetic studies. Bioorganic and Medicinal Chemistry, 2020, 28, 115467.	3.0	42
12	Synthesis, in vitro evaluation and molecular docking studies of biscoumarin thiourea as a new inhibitor of α-glucosidases. Bioorganic Chemistry, 2015, 63, 36-44.	4.1	41
13	Improved color stability of anthocyanins in the presence of ascorbic acid with the combination of rosmarinic acid and xanthan gum. Food Chemistry, 2021, 351, 129317.	8.2	40
14	New triazinoindole bearing thiazole/oxazole analogues: Synthesis, α-amylase inhibitory potential and molecular docking study. Bioorganic Chemistry, 2019, 92, 103284.	4.1	38
15	Synthesis, in vitro α-amylase inhibitory, and radicals (DPPH & ABTS) scavenging potentials of new N-sulfonohydrazide substituted indazoles. Bioorganic Chemistry, 2020, 94, 103410.	4.1	34
16	In-silico design of peptide inhibitors of K-Ras target in cancer disease. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5488-5499.	3.5	31
17	Synthesis and screening of (E)-3-(2-benzylidenehydrazinyl)-5,6-diphenyl-1,2,4-triazine analogs as novel dual inhibitors of α-amylase and α-glucosidase. Bioorganic Chemistry, 2020, 101, 103979.	4.1	29
18	Potent α-amylase inhibitors and radical (DPPH and ABTS) scavengers based on benzofuran-2-yl(phenyl)methanone derivatives: Syntheses, in vitro, kinetics, and in silico studies. Bioorganic Chemistry, 2020, 104, 104238.	4.1	23

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19	Natural compounds from plants controlling leishmanial growth via DNA damage and inhibiting trypanothione reductase and trypanothione synthetase: an in vitro and in silico approach. 3 Biotech, 2019, 9, 303.	2.2	14
20	Antihyperuricemic effect of dietary polyphenol sinapic acid commonly present in various edible food plants. Journal of Food Biochemistry, 2020, 44, e13111.	2.9	13
21	Dual roles of ATP-binding site in protein kinases: Orthosteric inhibition and allosteric regulation. Advances in Protein Chemistry and Structural Biology, 2021, 124, 87-119.	2.3	10
22	Predicting Multi-Interfacial Binding Mechanisms of NLRP3 and ASC Pyrin Domains in Inflammasome Activation. ACS Chemical Neuroscience, 2021, 12, 603-612.	3.5	10
23	<i>N</i> -Aryl-3,4-dihydroisoquinoline Carbothioamide Analogues as Potential Urease Inhibitors. ACS Omega, 2021, 6, 15794-15803.	3.5	9
24	Synthesis, <i>inÂvitro</i> biological screening and docking study of benzo[<i>d</i>]oxazole <i>bis</i> Schiff base derivatives as a potent anti-Alzheimer agent. Journal of Biomolecular Structure and Dynamics, 2023, 41, 1649-1664.	3.5	9
25	Dihydroquinazolin-4(1H)-one derivatives as novel and potential leads for diabetic management. Molecular Diversity, 2022, 26, 849-868.	3.9	7
26	Allosteric Modulation of Intrinsically Disordered Proteins. Advances in Experimental Medicine and Biology, 2019, 1163, 335-357.	1.6	7
27	Heparin-Assisted Amyloidogenesis Uncovered through Molecular Dynamics Simulations. ACS Omega, 2022, 7, 15132-15144.	3.5	7
28	Synthesis, urease inhibition screening and molecular docking studies of piperonal based imine derivatives. Medicinal Chemistry Research, 2021, 30, 226-235.	2.4	5
29	Strategies for Targeting KRAS: A Challenging Drug Target. Current Pharmaceutical Design, 2022, 28, 1897-1901.	1.9	4
30	Synthesis, characterization, in vitro biological and computational evaluation of 5-benzyl-4-(benzylideneamino)-2H-1,2,4-triazole-3(4H)-thiones. Journal of the Iranian Chemical Society, 2021, 18, 1965-1977.	2.2	3
31	Review on Pharmacological and Phytochemical Prospects of Traditional Medicinal Plant: Persicaria hydropiper (Smartweed). Current Topics in Medicinal Chemistry, 2021, 21, 1027-1036.	2.1	3
32	Toward the Noninvasive Diagnosis of Alzheimer's Disease: Molecular Basis for the Specificity of Curcumin for Fibrillar Amyloid-β. ACS Omega, 2022, 7, 22032-22038.	3.5	3
33	Computational Insight into the Binding Mechanism of Pyrazinoic Acid to RpsA Protein. Current Chinese Science, 2021, 1, 207-215.	0.5	2
34	A unique amphiphilic triblock copolymer, nontoxic to human blood and potential supramolecular drug delivery system for dexamethasone. Scientific Reports, 2021, 11, 21507.	3.3	2
35	A computational subtractive genome analysis for the characterization of novel drug targets in Klebsiella pneumonia strain PittNDM01. Microbial Pathogenesis, 2020, 146, 104245.	2.9	1
36	Disaggregation mechanism of prion amyloid for tweezer inhibitor. International Journal of Biological Macromolecules, 2021, 176, 510-519.	7.5	1