

Ashfaq Ur Rehman

List of Publications by Year in descending order

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36
papers

1,117
citations

430874

18
h-index

395702

33
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all docs

36
docs citations

36
times ranked

999
citing authors

#	ARTICLE	IF	CITATIONS
1	Synthesis, <i>in vitro</i> biological screening and docking study of benzo[d]oxazole bis Schiff base derivatives as a potent anti-Alzheimer agent. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 1649-1664.	3.5	9
2	Dihydroquinazolin-4(1H)-one derivatives as novel and potential leads for diabetic management. <i>Molecular Diversity</i> , 2022, 26, 849-868.	3.9	7
3	Heparin-Assisted Amyloidogenesis Uncovered through Molecular Dynamics Simulations. <i>ACS Omega</i> , 2022, 7, 15132-15144.	3.5	7
4	Strategies for Targeting KRAS: A Challenging Drug Target. <i>Current Pharmaceutical Design</i> , 2022, 28, 1897-1901.	1.9	4
5	Toward the Noninvasive Diagnosis of Alzheimer's Disease: Molecular Basis for the Specificity of Curcumin for Fibrillar Amyloid- β . <i>ACS Omega</i> , 2022, 7, 22032-22038.	3.5	3
6	Discovery of cryptic allosteric sites using reversed allosteric communication by a combined computational and experimental strategy. <i>Chemical Science</i> , 2021, 12, 464-476.	7.4	84
7	Synthesis, urease inhibition screening and molecular docking studies of piperonal based imine derivatives. <i>Medicinal Chemistry Research</i> , 2021, 30, 226-235.	2.4	5
8	Dual roles of ATP-binding site in protein kinases: Orthosteric inhibition and allosteric regulation. <i>Advances in Protein Chemistry and Structural Biology</i> , 2021, 124, 87-119.	2.3	10
9	Synthesis, characterization, <i>in vitro</i> biological and computational evaluation of 5-benzyl-4-(benzylideneamino)-2H-1,2,4-triazole-3(4H)-thiones. <i>Journal of the Iranian Chemical Society</i> , 2021, 18, 1965-1977.	2.2	3
10	Computational Insight into the Binding Mechanism of Pyrazinoic Acid to RpsA Protein. <i>Current Chinese Science</i> , 2021, 1, 207-215.	0.5	2
11	Disaggregation mechanism of prion amyloid for tweezer inhibitor. <i>International Journal of Biological Macromolecules</i> , 2021, 176, 510-519.	7.5	1
12	<i>N</i> -Aryl-3,4-dihydroisoquinoline Carbothioamide Analogues as Potential Urease Inhibitors. <i>ACS Omega</i> , 2021, 6, 15794-15803.	3.5	9
13	Improved color stability of anthocyanins in the presence of ascorbic acid with the combination of rosmarinic acid and xanthan gum. <i>Food Chemistry</i> , 2021, 351, 129317.	8.2	40
14	Review on Pharmacological and Phytochemical Prospects of Traditional Medicinal Plant: <i>Persicaria hydropiper</i> (Smartweed). <i>Current Topics in Medicinal Chemistry</i> , 2021, 21, 1027-1036.	2.1	3
15	Predicting Multi-Interfacial Binding Mechanisms of NLRP3 and ASC Pyrin Domains in Inflammasome Activation. <i>ACS Chemical Neuroscience</i> , 2021, 12, 603-612.	3.5	10
16	A unique amphiphilic triblock copolymer, nontoxic to human blood and potential supramolecular drug delivery system for dexamethasone. <i>Scientific Reports</i> , 2021, 11, 21507.	3.3	2
17	Synthesis of new indazole based dual inhibitors of α -glucosidase and α -amylase enzymes, their <i>in vitro</i> , <i>in silico</i> and kinetics studies. <i>Bioorganic Chemistry</i> , 2020, 94, 103195.	4.1	51
18	Synthesis, <i>in vitro</i> α -amylase inhibitory, and radicals (DPPH & ABTS) scavenging potentials of new <i>N</i> -sulfonohydrazide substituted indazoles. <i>Bioorganic Chemistry</i> , 2020, 94, 103410.	4.1	34

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19	Antihyperuricemic effect of dietary polyphenol sinapic acid commonly present in various edible food plants. <i>Journal of Food Biochemistry</i> , 2020, 44, e13111.	2.9	13
20	In-silico design of peptide inhibitors of K-Ras target in cancer disease. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 5488-5499.	3.5	31
21	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. <i>Bioorganic Chemistry</i> , 2020, 104, 104238.	4.1	23
22	A computational subtractive genome analysis for the characterization of novel drug targets in <i>Klebsiella pneumonia</i> strain PittNDM01. <i>Microbial Pathogenesis</i> , 2020, 146, 104245.	2.9	1
23	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. <i>Bioorganic Chemistry</i> , 2020, 101, 103979.	4.1	29
24	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. <i>Bioorganic and Medicinal Chemistry</i> , 2020, 28, 115467.	3.0	42
25	Synthesis of quinoline derivatives as diabetic II inhibitors and molecular docking studies. <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 4081-4088.	3.0	45
26	Natural compounds from plants controlling leishmanial growth via DNA damage and inhibiting trypanothione reductase and trypanothione synthetase: an in vitro and in silico approach. <i>3 Biotech</i> , 2019, 9, 303.	2.2	14
27	Synthesis of benzotriazoles derivatives and their dual potential as α -amylase and α -glucosidase inhibitors in vitro: Structure-activity relationship, molecular docking, and kinetic studies. <i>European Journal of Medicinal Chemistry</i> , 2019, 183, 111677.	5.5	78
28	New triazinoindole bearing thiazole/oxazole analogues: Synthesis, α -amylase inhibitory potential and molecular docking study. <i>Bioorganic Chemistry</i> , 2019, 92, 103284.	4.1	38
29	Synthesis, in vitro urease inhibitory potential and molecular docking study of Benzimidazole analogues. <i>Bioorganic Chemistry</i> , 2019, 89, 103024.	4.1	45
30	Structural and free energy landscape of novel mutations in ribosomal protein S1 (rpsA) associated with pyrazinamide resistance. <i>Scientific Reports</i> , 2019, 9, 7482.	3.3	48
31	Allosteric Modulation of Intrinsically Disordered Proteins. <i>Advances in Experimental Medicine and Biology</i> , 2019, 1163, 335-357.	1.6	7
32	Synthesis, α -glucosidase inhibitory, cytotoxicity and docking studies of 2-aryl-7-methylbenzimidazoles. <i>Bioorganic Chemistry</i> , 2016, 65, 100-109.	4.1	47
33	Novel quinoline derivatives as potent in vitro α -glucosidase inhibitors: in silico studies and SAR predictions. <i>MedChemComm</i> , 2015, 6, 1826-1836.	3.4	58
34	Isatin based Schiff bases as inhibitors of α -glucosidase: Synthesis, characterization, in vitro evaluation and molecular docking studies. <i>Bioorganic Chemistry</i> , 2015, 60, 42-48.	4.1	147
35	Synthesis, in vitro evaluation and molecular docking studies of biscoumarin thiourea as a new inhibitor of α -glucosidases. <i>Bioorganic Chemistry</i> , 2015, 63, 36-44.	4.1	41
36	Triazinoindole analogs as potent inhibitors of α -glucosidase: Synthesis, biological evaluation and molecular docking studies. <i>Bioorganic Chemistry</i> , 2015, 58, 81-87.	4.1	126