## Faez Iqbal Khan

List of Publications by Year in descending order

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186209 223716 2,353 68 28 46 citations h-index g-index papers 68 68 68 2517 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	The Lid Domain in Lipases: Structural and Functional Determinant of Enzymatic Properties. Frontiers in Bioengineering and Biotechnology, 2017, 5, 16.	2.0	243
2	X-ray photoelectron spectroscopic study of montmorillonite containing exchangeable divalent cations. Journal of the Chemical Society Faraday Transactions I, 1984, 80, 237.	1.0	149
3	Current updates on computer aided protein modeling and designing. International Journal of Biological Macromolecules, 2016, 85, 48-62.	3.6	123
4	Identification and evaluation of bioactive natural products as potential inhibitors of human microtubule affinity-regulating kinase 4 (MARK4). Journal of Biomolecular Structure and Dynamics, 2019, 37, 1813-1829.	2.0	114
5	A functional natural deep eutectic solvent based on trehalose: Structural and physicochemical properties. Food Chemistry, 2017, 217, 560-567.	4.2	99
6	Investigation of molecular mechanism of recognition between citral and MARK4: A newer therapeutic approach to attenuate cancer cell progression. International Journal of Biological Macromolecules, 2018, 107, 2580-2589.	3.6	96
7	Large scale analysis of the mutational landscape in $\hat{l}^2$ -glucuronidase: A major player of mucopolysaccharidosis type VII. Gene, 2016, 576, 36-44.	1.0	79
8	Identification and Evaluation of Inhibitors of Lipase from Malassezia restricta using Virtual High-Throughput Screening and Molecular Dynamics Studies. International Journal of Molecular Sciences, 2019, 20, 884.	1.8	72
9	Sleep Bruxism Detection Using Decision Tree Method by the Combination of C4-P4 and C4-A1 Channels of Scalp EEG. IEEE Access, 2019, 7, 102542-102553.	2.6	63
10	Role of N-terminal residues on folding and stability of C-phycoerythrin: simulation and urea-induced denaturation studies. Journal of Biomolecular Structure and Dynamics, 2015, 33, 121-133.	2.0	60
11	High throughput screening, docking, and molecular dynamics studies to identify potential inhibitors of human calcium/calmodulin-dependent protein kinase IV. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2179-2192.	2.0	60
12	Creation of thermostable and alkaline stable xylanase variants by DNA shuffling. Journal of Biotechnology, 2014, 187, 139-146.	1.9	57
13	Prognosis of Sleep Bruxism Using Power Spectral Density Approach Applied on EEG Signal of Both EMG1-EMG2 and ECG1-ECG2 Channels. IEEE Access, 2019, 7, 82553-82562.	2.6	55
14	Thermostable chitinase II from Thermomyces lanuginosus SSBP: Cloning, structure prediction and molecular dynamics simulations. Journal of Theoretical Biology, 2015, 374, 107-114.	0.8	53
15	Molecular mechanism of Ras-related protein Rab-5A and effect of mutations in the catalytically active phosphate-binding loop. Journal of Biomolecular Structure and Dynamics, 2017, 35, 105-118.	2.0	52
16	Binding mechanism of caffeic acid and simvastatin to the integrin linked kinase for therapeutic implications: a comparative docking and MD simulation studies. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4327-4337.	2.0	52
17	Cloning, expression, and molecular dynamics simulations of a xylosidase obtained from <i>Thermomyces lanuginosus </i> . Journal of Biomolecular Structure and Dynamics, 2016, 34, 1681-1692.	2.0	45
18	Implications of molecular diversity of chitin and its derivatives. Applied Microbiology and Biotechnology, 2017, 101, 3513-3536.	1.7	45

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19	Exploring molecular insights into the interaction mechanism of cholesterol derivatives with the Mce4A: A combined spectroscopic and molecular dynamic simulation studies. International Journal of Biological Macromolecules, 2018, 111, 548-560.	3.6	45
20	Crystal structure of a lipase from <i>Streptomyces</i> sp. strain W007 – implications for thermostability and regiospecificity. FEBS Journal, 2017, 284, 3506-3519.	2.2	44
21	Functional implications of pH-induced conformational changes in the Sphingosine kinase 1. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 225, 117453.	2.0	44
22	Chitinase from Thermomyces lanuginosus SSBP and its biotechnological applications. Extremophiles, 2015, 19, 1055-1066.	0.9	42
23	Elucidation of interaction mechanism of ellagic acid to the integrin linked kinase. International Journal of Biological Macromolecules, 2019, 122, 1297-1304.	3.6	38
24	Structure prediction and functional analyses of a thermostable lipase obtained from Shewanella putrefaciens. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2123-2135.	2.0	34
25	Mitochondrial Dynamics and Proteins Related to Neurodegenerative Diseases. Current Protein and Peptide Science, 2018, 19, 850-857.	0.7	34
26	Remdesivir Strongly Binds to RNA-Dependent RNA Polymerase, Membrane Protein, and Main Protease of SARS-CoV-2: Indication From Molecular Modeling and Simulations. Frontiers in Pharmacology, 2021, 12, 710778.	1.6	33
27	Mechanistic insights into the urea-induced denaturation of kinase domain of human integrin linked kinase. International Journal of Biological Macromolecules, 2018, 111, 208-218.	3.6	31
28	Pyrazoline analogs as potential anticancer agents and their apoptosis, molecular docking, MD simulation, DNA binding and antioxidant studies. Bioorganic Chemistry, 2021, 108, 104665.	2.0	31
29	Identifying novel sphingosine kinase 1 inhibitors as therapeutics against breast cancer. Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 172-186.	2.5	28
30	Sequence Analysis of Hypothetical Proteins from <i>Helicobacter pylori</i> Virulence Factors. Genomics and Informatics, 2016, 14, 125.	0.4	28
31	Seed Extract of Psoralea corylifolia and Its Constituent Bakuchiol Impairs AHL-Based Quorum Sensing and Biofilm Formation in Food- and Human-Related Pathogens. Frontiers in Cellular and Infection Microbiology, 2018, 8, 351.	1.8	27
32	Human serum albumin interaction, in silico and anticancer evaluation of Pine-Gold nanoparticles. Process Biochemistry, 2020, 89, 98-109.	1.8	27
33	An In Vitro elucidation of the antiaggregatory potential of Diosminover thermally induced unfolding of hen egg white lysozyme; A preventive quest for lysozyme amyloidosis. International Journal of Biological Macromolecules, 2019, 129, 1015-1023.	3.6	20
34	Fate of T Cells and their Secretory Proteins During the Progression of Leprosy. Current Protein and Peptide Science, 2018, 19, 889-899.	0.7	19
35	Pressure induced superconductivity and electronic structure properties of scandium hydrides using first principles calculations. RSC Advances, 2016, 6, 81534-81541.	1.7	17
36	Unravelling the unfolding mechanism of human integrin linked kinase by GdmCl-induced denaturation. International Journal of Biological Macromolecules, 2018, 117, 1252-1263.	3.6	15

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37	In silico studies and evaluation of antiparasitic role of a novel pyruvate phosphate dikinase inhibitor in Leishmania donovani infected macrophages. International Journal of Antimicrobial Agents, 2019, 53, 508-514.	1.1	15
38	A Thermolabile Phospholipase B from Talaromyces marneffei GD-0079: Biochemical Characterization and Structure Dynamics Study. Biomolecules, 2020, 10, 231.	1.8	15
39	A comparative study on kinetics and substrate specificities of Phospholipase A1 with Thermomyces lanuginosus lipase. Journal of Colloid and Interface Science, 2017, 488, 149-154.	5.0	14
40	Recent Studies of Mitochondrial SLC25: Integration of Experimental and Computational Approaches. Current Protein and Peptide Science, 2018, 19, 507-522.	0.7	14
41	Mechanistic insights into the urea-induced denaturation of human sphingosine kinase 1. International Journal of Biological Macromolecules, 2020, 161, 1496-1505.	3.6	14
42	Comparative Analysis of Bacteriophytochrome Agp2 and Its Engineered Photoactivatable NIR Fluorescent Proteins PAiRFP1 and PAiRFP2. Biomolecules, 2020, 10, 1286.	1.8	14
43	Malassezia globosa Mg MDL2 lipase: Crystal structure and rational modification of substrate specificity. Biochemical and Biophysical Research Communications, 2017, 488, 259-265.	1.0	13
44	QSAR based therapeutic management of M. tuberculosis. Archives of Pharmacal Research, 2017, 40, 676-694.	2.7	13
45	Probing pH sensitivity of $\hat{i}$ ±C-phycoerythrin and its natural truncant: A comparative study. International Journal of Biological Macromolecules, 2016, 86, 18-27.	3.6	12
46	Investigation of guanidinium chloride-induced unfolding pathway of sphingosine kinase 1. International Journal of Biological Macromolecules, 2020, 147, 177-186.	3.6	12
47	In Silico Studies on Psilocybin Drug Derivatives Against SARS-CoV-2 and Cytokine Storm of Human Interleukin-6 Receptor. Frontiers in Immunology, 2021, 12, 794780.	2.2	12
48	Siteâ€directed mutagenesis studies of hydrophobic residues in the lid region of T1 lipase. European Journal of Lipid Science and Technology, 2017, 119, 1600107.	1.0	11
49	Effects of reverse genetic mutations on the spectral and photochemical behavior of a photoactivatable fluorescent protein PAiRFP1. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 228, 117807.	2.0	11
50	Investigating the binding mechanism of topiramate with bovine serum albumin using spectroscopic and computational methods. Journal of Molecular Recognition, 2022, 35, e2958.	1.1	11
51	Impact of amino acid substitutions on the behavior of a photoactivatable near infrared fluorescent protein PAiRFP1. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 253, 119572.	2.0	10
52	Mechanistic insights into the urea-induced denaturation of a non-seleno thiol specific antioxidant human peroxiredoxin 6. International Journal of Biological Macromolecules, 2020, 161, 1171-1180.	3.6	9
53	<i>In silico</i> prediction of natural compounds as potential multi-target inhibitors of structural proteins of SARS-CoV-2. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12118-12134.	2.0	9
54	Molecular dynamics simulation of chitinase I from <i>Thermomyces lanuginosus SSBP</i> to ensure optimal activity. Molecular Simulation, 2017, 43, 480-490.	0.9	8

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55	High-resolution MD Simulation Studies to Get Mechanistic Insights into the Urea-induced Denaturation of Human Sphingosine Kinase 1. Current Topics in Medicinal Chemistry, 2021, 21, 2839-2850.	1.0	8
56	Profiling substrate specificity of Lecitase Ultra to different kinds of phospholipids using monolayer technology. European Journal of Lipid Science and Technology, 2017, 119, 1600175.	1.0	6
57	Mechanism of pH-induced conformational changes in MurE ligase obtained from <i>Salmonella enterica</i> serovar Typhi. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1898-1905.	2.0	6
58	The Molecular Basis of the Effect of Temperature on the Structure and Function of SARS-CoV-2 Spike Protein. Frontiers in Molecular Biosciences, 2022, 9, 794960.	1.6	6
59	Diacylglycerol production by genetically modified lipase from Malassezia globosa. Journal of Molecular Catalysis B: Enzymatic, 2016, 133, S204-S212.	1.8	5
60	Open and closed states of Mrlip1 DAG lipase revealed by molecular dynamics simulation. Molecular Simulation, 2018, 44, 1520-1528.	0.9	5
61	Green Synthesis, Experimental and Theoretical Studies to Discover Novel Binders of Exosomal Tetraspanin CD81 Protein. ACS Omega, 2020, 5, 17973-17982.	1.6	5
62	Effect of polyol osmolytes on the structure-function integrity and aggregation propensity of catalase: A comprehensive study based on spectroscopic and molecular dynamic simulation measurements. International Journal of Biological Macromolecules, 2022, 209, 198-210.	3.6	5
63	Chloroacetaldehyde dehydrogenase from Ancylobacter aquaticus UV5: Cloning, expression, characterization and molecular modeling. International Journal of Biological Macromolecules, 2018, 114, 1117-1126.	3.6	4
64	From Pancreatic to Non-Pancreatic Insulin: A Miraculous Journey. International Journal of Biological Chemistry, 2015, 9, 302-317.	0.3	4
65	A pH based molecular dynamics simulations of chitinase II isolated from Thermomyces lanuginosus SSBP. Cogent Biology, 2016, 2, 1168336.	1.7	3
66	Substrate selectivity and optimization of immobilized SMG1â€F278N lipase in synthesis of propylene glycol monooleate. European Journal of Lipid Science and Technology, 2017, 119, 1600423.	1.0	3
67	Improving phospholipase activity of PLA $<$ sub $>1sub> by protein engineering and its effects on oil degumming. European Journal of Lipid Science and Technology, 2017, 119, 1600110.$	1.0	2
68	Addition of Mercury Causes Quenching of NIR Fluorescence Emission Spectra of a Photoactivatable PAiRFP1 Protein. Current Protein and Peptide Science, 2022, 23, .	0.7	0