

# Faez Iqbal Khan

## List of Publications by Year in descending order

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Version: 2024-02-01

68  
papers

2,353  
citations

186209

28  
h-index

223716

46  
g-index

68  
all docs

68  
docs citations

68  
times ranked

2517  
citing authors

#	ARTICLE	IF	CITATIONS
1	<i>In silico</i> prediction of natural compounds as potential multi-target inhibitors of structural proteins of SARS-CoV-2. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 12118-12134.	2.0	9
2	The Molecular Basis of the Effect of Temperature on the Structure and Function of SARS-CoV-2 Spike Protein. <i>Frontiers in Molecular Biosciences</i> , 2022, 9, 794960.	1.6	6
3	Investigating the binding mechanism of topiramate with bovine serum albumin using spectroscopic and computational methods. <i>Journal of Molecular Recognition</i> , 2022, 35, e2958.	1.1	11
4	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. <i>International Journal of Biological Macromolecules</i> , 2022, 209, 198-210.	3.6	5
5	Addition of Mercury Causes Quenching of NIR Fluorescence Emission Spectra of a Photoactivatable PAiRFP1 Protein. <i>Current Protein and Peptide Science</i> , 2022, 23, .	0.7	0
6	Mechanism of pH-induced conformational changes in MurE ligase obtained from <i>Salmonella enterica</i> serovar Typhi. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 1898-1905.	2.0	6
7	Pyrazoline analogs as potential anticancer agents and their apoptosis, molecular docking, MD simulation, DNA binding and antioxidant studies. <i>Bioorganic Chemistry</i> , 2021, 108, 104665.	2.0	31
8	Impact of amino acid substitutions on the behavior of a photoactivatable near infrared fluorescent protein PAiRFP1. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 253, 119572.	2.0	10
9	Remdesivir Strongly Binds to RNA-Dependent RNA Polymerase, Membrane Protein, and Main Protease of SARS-CoV-2: Indication From Molecular Modeling and Simulations. <i>Frontiers in Pharmacology</i> , 2021, 12, 710778.	1.6	33
10	High-resolution MD Simulation Studies to Get Mechanistic Insights into the Urea-induced Denaturation of Human Sphingosine Kinase 1. <i>Current Topics in Medicinal Chemistry</i> , 2021, 21, 2839-2850.	1.0	8
11	<i>In Silico</i> Studies on Psilocybin Drug Derivatives Against SARS-CoV-2 and Cytokine Storm of Human Interleukin-6 Receptor. <i>Frontiers in Immunology</i> , 2021, 12, 794780.	2.2	12
12	Human serum albumin interaction, <i>in silico</i> and anticancer evaluation of Pine-Gold nanoparticles. <i>Process Biochemistry</i> , 2020, 89, 98-109.	1.8	27
13	Functional implications of pH-induced conformational changes in the Sphingosine kinase 1. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 225, 117453.	2.0	44
14	Investigation of guanidinium chloride-induced unfolding pathway of sphingosine kinase 1. <i>International Journal of Biological Macromolecules</i> , 2020, 147, 177-186.	3.6	12
15	Effects of reverse genetic mutations on the spectral and photochemical behavior of a photoactivatable fluorescent protein PAiRFP1. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 228, 117807.	2.0	11
16	Identifying novel sphingosine kinase 1 inhibitors as therapeutics against breast cancer. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2020, 35, 172-186.	2.5	28
17	Mechanistic insights into the urea-induced denaturation of human sphingosine kinase 1. <i>International Journal of Biological Macromolecules</i> , 2020, 161, 1496-1505.	3.6	14
18	Green Synthesis, Experimental and Theoretical Studies to Discover Novel Binders of Exosomal Tetraspanin CD81 Protein. <i>ACS Omega</i> , 2020, 5, 17973-17982.	1.6	5

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19	Comparative Analysis of Bacteriophytochrome Agp2 and Its Engineered Photoactivatable NIR Fluorescent Proteins PAiRFP1 and PAiRFP2. <i>Biomolecules</i> , 2020, 10, 1286.	1.8	14
20	Mechanistic insights into the urea-induced denaturation of a non-seleno thiol specific antioxidant human peroxiredoxin 6. <i>International Journal of Biological Macromolecules</i> , 2020, 161, 1171-1180.	3.6	9
21	A Thermolabile Phospholipase B from <i>Talaromyces marneffei</i> GD-0079: Biochemical Characterization and Structure Dynamics Study. <i>Biomolecules</i> , 2020, 10, 231.	1.8	15
22	High throughput screening, docking, and molecular dynamics studies to identify potential inhibitors of human calcium/calmodulin-dependent protein kinase IV. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 2179-2192.	2.0	60
23	Sleep Bruxism Detection Using Decision Tree Method by the Combination of C4-P4 and C4-A1 Channels of Scalp EEG. <i>IEEE Access</i> , 2019, 7, 102542-102553.	2.6	63
24	Prognosis of Sleep Bruxism Using Power Spectral Density Approach Applied on EEG Signal of Both EMG1-EMG2 and ECG1-ECG2 Channels. <i>IEEE Access</i> , 2019, 7, 82553-82562.	2.6	55
25	An In Vitro elucidation of the antiaggregatory potential of Diosmin over thermally induced unfolding of hen egg white lysozyme; A preventive quest for lysozyme amyloidosis. <i>International Journal of Biological Macromolecules</i> , 2019, 129, 1015-1023.	3.6	20
26	Identification and Evaluation of Inhibitors of Lipase from <i>Malassezia restricta</i> using Virtual High-Throughput Screening and Molecular Dynamics Studies. <i>International Journal of Molecular Sciences</i> , 2019, 20, 884.	1.8	72
27	Elucidation of interaction mechanism of ellagic acid to the integrin linked kinase. <i>International Journal of Biological Macromolecules</i> , 2019, 122, 1297-1304.	3.6	38
28	In silico studies and evaluation of antiparasitic role of a novel pyruvate phosphate dikinase inhibitor in <i>Leishmania donovani</i> infected macrophages. <i>International Journal of Antimicrobial Agents</i> , 2019, 53, 508-514.	1.1	15
29	Binding mechanism of caffeic acid and simvastatin to the integrin linked kinase for therapeutic implications: a comparative docking and MD simulation studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 4327-4337.	2.0	52
30	Identification and evaluation of bioactive natural products as potential inhibitors of human microtubule affinity-regulating kinase 4 (MARK4). <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 1813-1829.	2.0	114
31	Chloroacetaldehyde dehydrogenase from <i>Ancylobacter aquaticus</i> UV5: Cloning, expression, characterization and molecular modeling. <i>International Journal of Biological Macromolecules</i> , 2018, 114, 1117-1126.	3.6	4
32	Exploring molecular insights into the interaction mechanism of cholesterol derivatives with the Mce4A: A combined spectroscopic and molecular dynamic simulation studies. <i>International Journal of Biological Macromolecules</i> , 2018, 111, 548-560.	3.6	45
33	Mechanistic insights into the urea-induced denaturation of kinase domain of human integrin linked kinase. <i>International Journal of Biological Macromolecules</i> , 2018, 111, 208-218.	3.6	31
34	Investigation of molecular mechanism of recognition between citral and MARK4: A newer therapeutic approach to attenuate cancer cell progression. <i>International Journal of Biological Macromolecules</i> , 2018, 107, 2580-2589.	3.6	96
35	Seed Extract of <i>Psoralea corylifolia</i> and Its Constituent Bakuchiol Impairs AHL-Based Quorum Sensing and Biofilm Formation in Food- and Human-Related Pathogens. <i>Frontiers in Cellular and Infection Microbiology</i> , 2018, 8, 351.	1.8	27
36	Open and closed states of Mrlip1 DAG lipase revealed by molecular dynamics simulation. <i>Molecular Simulation</i> , 2018, 44, 1520-1528.	0.9	5

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37	Recent Studies of Mitochondrial SLC25: Integration of Experimental and Computational Approaches. <i>Current Protein and Peptide Science</i> , 2018, 19, 507-522.	0.7	14
38	Unravelling the unfolding mechanism of human integrin linked kinase by GdmCl-induced denaturation. <i>International Journal of Biological Macromolecules</i> , 2018, 117, 1252-1263.	3.6	15
39	Mitochondrial Dynamics and Proteins Related to Neurodegenerative Diseases. <i>Current Protein and Peptide Science</i> , 2018, 19, 850-857.	0.7	34
40	Fate of T Cells and their Secretory Proteins During the Progression of Leprosy. <i>Current Protein and Peptide Science</i> , 2018, 19, 889-899.	0.7	19
41	Molecular mechanism of Ras-related protein Rab-5A and effect of mutations in the catalytically active phosphate-binding loop. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017, 35, 105-118.	2.0	52
42	Improving phospholipase activity of PLA <sub>1</sub> by protein engineering and its effects on oil degumming. <i>European Journal of Lipid Science and Technology</i> , 2017, 119, 1600110.	1.0	2
43	Site-directed mutagenesis studies of hydrophobic residues in the lid region of T1 lipase. <i>European Journal of Lipid Science and Technology</i> , 2017, 119, 1600107.	1.0	11
44	Structure prediction and functional analyses of a thermostable lipase obtained from <i>Shewanella putrefaciens</i> . <i>Journal of Biomolecular Structure and Dynamics</i> , 2017, 35, 2123-2135.	2.0	34
45	Substrate selectivity and optimization of immobilized SMG1 $\epsilon$ 278N lipase in synthesis of propylene glycol monooleate. <i>European Journal of Lipid Science and Technology</i> , 2017, 119, 1600423.	1.0	3
46	<i>Malassezia globosa</i> Mg MDL2 lipase: Crystal structure and rational modification of substrate specificity. <i>Biochemical and Biophysical Research Communications</i> , 2017, 488, 259-265.	1.0	13
47	QSAR based therapeutic management of <i>M. tuberculosis</i> . <i>Archives of Pharmacal Research</i> , 2017, 40, 676-694.	2.7	13
48	Implications of molecular diversity of chitin and its derivatives. <i>Applied Microbiology and Biotechnology</i> , 2017, 101, 3513-3536.	1.7	45
49	Crystal structure of a lipase from <i>Streptomyces</i> sp. strain W007 – implications for thermostability and regiospecificity. <i>FEBS Journal</i> , 2017, 284, 3506-3519.	2.2	44
50	A comparative study on kinetics and substrate specificities of Phospholipase A1 with <i>Thermomyces lanuginosus</i> lipase. <i>Journal of Colloid and Interface Science</i> , 2017, 488, 149-154.	5.0	14
51	Profiling substrate specificity of Lecitase Ultra to different kinds of phospholipids using monolayer technology. <i>European Journal of Lipid Science and Technology</i> , 2017, 119, 1600175.	1.0	6
52	Molecular dynamics simulation of chitinase I from <i>Thermomyces lanuginosus</i> SSBP to ensure optimal activity. <i>Molecular Simulation</i> , 2017, 43, 480-490.	0.9	8
53	A functional natural deep eutectic solvent based on trehalose: Structural and physicochemical properties. <i>Food Chemistry</i> , 2017, 217, 560-567.	4.2	99
54	The Lid Domain in Lipases: Structural and Functional Determinant of Enzymatic Properties. <i>Frontiers in Bioengineering and Biotechnology</i> , 2017, 5, 16.	2.0	243

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55	Diacylglycerol production by genetically modified lipase from <i>Malassezia globosa</i> . <i>Journal of Molecular Catalysis B: Enzymatic</i> , 2016, 133, S204-S212.	1.8	5
56	A pH based molecular dynamics simulations of chitinase II isolated from <i>Thermomyces lanuginosus</i> SSBP. <i>Cogent Biology</i> , 2016, 2, 1168336.	1.7	3
57	Pressure induced superconductivity and electronic structure properties of scandium hydrides using first principles calculations. <i>RSC Advances</i> , 2016, 6, 81534-81541.	1.7	17
58	Probing pH sensitivity of $\hat{1}\pm$ C-phycoerythrin and its natural truncant: A comparative study. <i>International Journal of Biological Macromolecules</i> , 2016, 86, 18-27.	3.6	12
59	Current updates on computer aided protein modeling and designing. <i>International Journal of Biological Macromolecules</i> , 2016, 85, 48-62.	3.6	123
60	Large scale analysis of the mutational landscape in $\hat{1}^2$ -glucuronidase: A major player of mucopolysaccharidosis type VII. <i>Gene</i> , 2016, 576, 36-44.	1.0	79
61	Cloning, expression, and molecular dynamics simulations of a xylosidase obtained from <i>Thermomyces lanuginosus</i> . <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 1681-1692.	2.0	45
62	Sequence Analysis of Hypothetical Proteins from <i>Helicobacter pylori</i> 26695 to Identify Potential Virulence Factors. <i>Genomics and Informatics</i> , 2016, 14, 125.	0.4	28
63	Role of N-terminal residues on folding and stability of C-phycoerythrin: simulation and urea-induced denaturation studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 121-133.	2.0	60
64	Thermostable chitinase II from <i>Thermomyces lanuginosus</i> SSBP: Cloning, structure prediction and molecular dynamics simulations. <i>Journal of Theoretical Biology</i> , 2015, 374, 107-114.	0.8	53
65	Chitinase from <i>Thermomyces lanuginosus</i> SSBP and its biotechnological applications. <i>Extremophiles</i> , 2015, 19, 1055-1066.	0.9	42
66	From Pancreatic to Non-Pancreatic Insulin: A Miraculous Journey. <i>International Journal of Biological Chemistry</i> , 2015, 9, 302-317.	0.3	4
67	Creation of thermostable and alkaline stable xylanase variants by DNA shuffling. <i>Journal of Biotechnology</i> , 2014, 187, 139-146.	1.9	57
68	X-ray photoelectron spectroscopic study of montmorillonite containing exchangeable divalent cations. <i>Journal of the Chemical Society Faraday Transactions I</i> , 1984, 80, 237.	1.0	149