Nicholas Furnham

List of Publications by Year
in descending order

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Version: 2024-02-01

46 papers	2,965 citations	201674 27 h-index	223800 46 g-index
48 all docs	48 docs citations	48 times ranked	4741 citing authors

#	Article	IF	Citations
1	CATH: comprehensive structural and functional annotations for genome sequences. Nucleic Acids Research, 2015, 43, D376-D381.	14.5	399
2	Genome-wide analysis of multi- and extensively drug-resistant Mycobacterium tuberculosis. Nature Genetics, 2018, 50, 307-316.	21.4	271
3	New functional families (FunFams) in CATH to improve the mapping of conserved functional sites to 3D structures. Nucleic Acids Research, 2012, 41, D490-D498.	14.5	188
4	The Catalytic Site Atlas 2.0: cataloging catalytic sites and residues identified in enzymes. Nucleic Acids Research, 2014, 42, D485-D489.	14.5	168
5	Assembly and Channel Opening in a Bacterial Drug Efflux Machine. Molecular Cell, 2008, 30, 114-121.	9.7	155
6	Mechanism and Catalytic Site Atlas (M-CSA): a database of enzyme reaction mechanisms and active sites. Nucleic Acids Research, 2018, 46, D618-D623.	14.5	151
7	Extending CATH: increasing coverage of the protein structure universe and linking structure with function. Nucleic Acids Research, 2011, 39, D420-D426.	14.5	126
8	In silico Strategies to Support Fragment-to-Lead Optimization in Drug Discovery. Frontiers in Chemistry, 2020, 8, 93.	3.6	122
9	EC-BLAST: a tool to automatically search and compare enzyme reactions. Nature Methods, 2014, 11, 171-174.	19.0	112
10	Is one solution good enough?. Nature Structural and Molecular Biology, 2006, 13, 184-185.	8.2	110
11	The Classification and Evolution of Enzyme Function. Biophysical Journal, 2015, 109, 1082-1086.	0.5	95
12	Exploring the Evolution of Novel Enzyme Functions within Structurally Defined Protein Superfamilies. PLoS Computational Biology, 2012, 8, e1002403.	3.2	80
13	Chopping and Changing: the Evolution of the Flavin-dependent Monooxygenases. Journal of Molecular Biology, 2016, 428, 3131-3146.	4.2	75
14	Discovery of New Anti-Schistosomal Hits by Integration of QSAR-Based Virtual Screening and High Content Screening. Journal of Medicinal Chemistry, 2016, 59, 7075-7088.	6.4	67
15	Understanding molecular consequences of putative drug resistant mutations in Mycobacterium tuberculosis. Scientific Reports, 2018, 8, 15356.	3.3	64
16	Structure of an Xrcc4â€“DNA ligase IV yeast ortholog complex reveals a novel BRCT interaction mode. DNA Repair, 2006, 5, 362-368.	2.8	60
17	Large-Scale Analysis Exploring Evolution of Catalytic Machineries and Mechanisms in Enzyme Superfamilies. Journal of Molecular Biology, 2016, 428, 253-267.	4.2	55
18	To what extent do structural changes in catalytic metal sites affect enzyme function?. Journal of Inorganic Biochemistry, 2018, 179, 40-53.	3.5	55

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19	Missing in action: enzyme functional annotations in biological databases. Nature Chemical Biology, 2009, 5, 521-525.	8.0	53
20	QSAR-Driven Discovery of Novel Chemical Scaffolds Active against Schistosoma mansoni. Journal of Chemical Information and Modeling, 2016, 56, 1357-1372.	5.4	47
21	FunTree: a resource for exploring the functional evolution of structurally defined enzyme superfamilies. Nucleic Acids Research, 2012, 40, D776-D782.	14.5	44
22	Comparisons of Allergenic and Metazoan Parasite Proteins: Allergy the Price of Immunity. PLoS Computational Biology, 2015, 11, e1004546.	3.2	43
23	Structural basis for inhibition of homologous recombination by the RecX protein. EMBO Journal, 2008, 27, 2259-2269.	7.8	41
24	Understanding enzyme function evolution from a computational perspective. Current Opinion in Structural Biology, 2017, 47, 131-139.	5.7	36
25	The evolution of enzyme function in the isomerases. Current Opinion in Structural Biology, 2014, 26, 121-130.	5.7	33
26	Prediction of rifampicin resistance beyond the RRDR using structure-based machine learning approaches. Scientific Reports, 2020, 10, 18120.	3.3	30
27	Computationally-guided drug repurposing enables the discovery of kinase targets and inhibitors as new schistosomicidal agents. PLoS Computational Biology, 2018, 14, e1006515.	3.2	29
28	Structure and Mechanism of Drug Efflux Machinery in Gram Negative Bacteria. Current Drug Targets, 2008, 9, 719-728.	2.1	28
29	Knowledge-Based Real-Space Explorations for Low-Resolution Structure Determination. Structure, 2006, 14, 1313-1320.	3.3	27
30	Known Allergen Structures Predict Schistosoma mansoni IgE-Binding Antigens in Human Infection. Frontiers in Immunology, 2015, 6, 26.	4.8	25
31	Conformer generation under restraints. Current Opinion in Structural Biology, 2006, 16, 160-165.	5.7	24
32	Model-building strategies for low-resolution X-ray crystallographic data. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 121-127.	2.5	19
33	THE RAMACHANDRAN PLOT AND PROTEIN STRUCTURE VALIDATION. , 2013, , 62-75.		19
34	Combining structure and genomics to understand antimicrobial resistance. Computational and Structural Biotechnology Journal, 2020, 18, 3377-3394.	4.1	17
35	Unveiling the Kinomes of Leishmania infantum and L. braziliensis Empowers the Discovery of New Kinase Targets and Antileishmanial Compounds. Computational and Structural Biotechnology Journal, 2019, 17, 352-361.	4.1	16
36	Current challenges in genome annotation through structural biology and bioinformatics. Current Opinion in Structural Biology, 2012, 22, 594-601.	5.7	14

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37	FunTree: advances in a resource for exploring and contextualising protein function evolution. Nucleic Acids Research, 2016, 44, D317-D323.	14.5	13
38	Exploring the Biological and Chemical Complexity of the Ligases. Journal of Molecular Biology, 2014, 426, 2098-2111.	4.2	11
39	Schistosomiasis Drug Discovery in the Era of Automation and Artificial Intelligence. Frontiers in Immunology, 2021, 12, 642383.	4.8	10
40	Comparative modelling by restraint-based conformational sampling. BMC Structural Biology, 2008, 8, 7.	2.3	8
41	Exploring Enzyme Evolution from Changes in Sequence, Structure, and Function. Methods in Molecular Biology, 2019, 1851, 263-275.	0.9	8
42	Abstracting knowledge from the protein data bank. Biopolymers, 2013, 99, 183-188.	2.4	6
43	Chemogenomics and bioinformatics approaches for prioritizing kinases as drug targets for neglected tropical diseases. Advances in Protein Chemistry and Structural Biology, 2021, 124, 187-223.	2.3	2
44	Structural and Genomic Insights Into Pyrazinamide Resistance in Mycobacterium tuberculosis Underlie Differences Between Ancient and Modern Lineages. Frontiers in Molecular Biosciences, 2021, 8, 619403.	3.5	2
45	The complex relationship between the emerging flaviviruses: dengue and Zika. Biochemist, 2017, 39, 18-21.	0.5	1
46	Complementary Sources of Protein Functional Information: The Far Side of GO. Methods in Molecular Biology, 2017, 1446, 263-274.	0.9	1