

# 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	Chemogenomics and bioinformatics approaches for prioritizing kinases as drug targets for neglected tropical diseases. <i>Advances in Protein Chemistry and Structural Biology</i> , 2021, 124, 187-223.	2.3	2
2	Schistosomiasis Drug Discovery in the Era of Automation and Artificial Intelligence. <i>Frontiers in Immunology</i> , 2021, 12, 642383.	4.8	10
3	Structural and Genomic Insights Into Pyrazinamide Resistance in <i>Mycobacterium tuberculosis</i> Underlie Differences Between Ancient and Modern Lineages. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 619403.	3.5	2
4	Prediction of rifampicin resistance beyond the RRDR using structure-based machine learning approaches. <i>Scientific Reports</i> , 2020, 10, 18120.	3.3	30
5	Combining structure and genomics to understand antimicrobial resistance. <i>Computational and Structural Biotechnology Journal</i> , 2020, 18, 3377-3394.	4.1	17
6	In silico Strategies to Support Fragment-to-Lead Optimization in Drug Discovery. <i>Frontiers in Chemistry</i> , 2020, 8, 93.	3.6	122
7	Unveiling the Kinomes of <i>Leishmania infantum</i> and <i>L. braziliensis</i> Empowers the Discovery of New Kinase Targets and Antileishmanial Compounds. <i>Computational and Structural Biotechnology Journal</i> , 2019, 17, 352-361.	4.1	16
8	Exploring Enzyme Evolution from Changes in Sequence, Structure, and Function. <i>Methods in Molecular Biology</i> , 2019, 1851, 263-275.	0.9	8
9	Mechanism and Catalytic Site Atlas (M-CSA): a database of enzyme reaction mechanisms and active sites. <i>Nucleic Acids Research</i> , 2018, 46, D618-D623.	14.5	151
10	Genome-wide analysis of multi- and extensively drug-resistant <i>Mycobacterium tuberculosis</i> . <i>Nature Genetics</i> , 2018, 50, 307-316.	21.4	271
11	To what extent do structural changes in catalytic metal sites affect enzyme function?. <i>Journal of Inorganic Biochemistry</i> , 2018, 179, 40-53.	3.5	55
12	Computationally-guided drug repurposing enables the discovery of kinase targets and inhibitors as new schistosomicidal agents. <i>PLoS Computational Biology</i> , 2018, 14, e1006515.	3.2	29
13	Understanding molecular consequences of putative drug resistant mutations in <i>Mycobacterium tuberculosis</i> . <i>Scientific Reports</i> , 2018, 8, 15356.	3.3	64
14	Understanding enzyme function evolution from a computational perspective. <i>Current Opinion in Structural Biology</i> , 2017, 47, 131-139.	5.7	36
15	The complex relationship between the emerging flaviviruses: dengue and Zika. <i>Biochemist</i> , 2017, 39, 18-21.	0.5	1
16	Complementary Sources of Protein Functional Information: The Far Side of GO. <i>Methods in Molecular Biology</i> , 2017, 1446, 263-274.	0.9	1
17	Discovery of New Anti-Schistosomal Hits by Integration of QSAR-Based Virtual Screening and High Content Screening. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 7075-7088.	6.4	67
18	FunTree: advances in a resource for exploring and contextualising protein function evolution. <i>Nucleic Acids Research</i> , 2016, 44, D317-D323.	14.5	13

#	ARTICLE	IF	CITATIONS
19	Chopping and Changing: the Evolution of the Flavin-dependent Monooxygenases. <i>Journal of Molecular Biology</i> , 2016, 428, 3131-3146.	4.2	75
20	QSAR-Driven Discovery of Novel Chemical Scaffolds Active against <i>Schistosoma mansoni</i> . <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1357-1372.	5.4	47
21	Large-Scale Analysis Exploring Evolution of Catalytic Machineries and Mechanisms in Enzyme Superfamilies. <i>Journal of Molecular Biology</i> , 2016, 428, 253-267.	4.2	55
22	The Classification and Evolution of Enzyme Function. <i>Biophysical Journal</i> , 2015, 109, 1082-1086.	0.5	95
23	CATH: comprehensive structural and functional annotations for genome sequences. <i>Nucleic Acids Research</i> , 2015, 43, D376-D381.	14.5	399
24	Known Allergen Structures Predict <i>Schistosoma mansoni</i> IgE-Binding Antigens in Human Infection. <i>Frontiers in Immunology</i> , 2015, 6, 26.	4.8	25
25	Comparisons of Allergenic and Metazoan Parasite Proteins: Allergy the Price of Immunity. <i>PLoS Computational Biology</i> , 2015, 11, e1004546.	3.2	43
26	The Catalytic Site Atlas 2.0: cataloging catalytic sites and residues identified in enzymes. <i>Nucleic Acids Research</i> , 2014, 42, D485-D489.	14.5	168
27	The evolution of enzyme function in the isomerases. <i>Current Opinion in Structural Biology</i> , 2014, 26, 121-130.	5.7	33
28	EC-BLAST: a tool to automatically search and compare enzyme reactions. <i>Nature Methods</i> , 2014, 11, 171-174.	19.0	112
29	Exploring the Biological and Chemical Complexity of the Ligases. <i>Journal of Molecular Biology</i> , 2014, 426, 2098-2111.	4.2	11
30	Abstracting knowledge from the protein data bank. <i>Biopolymers</i> , 2013, 99, 183-188.	2.4	6
31	THE RAMACHANDRAN PLOT AND PROTEIN STRUCTURE VALIDATION. , 2013 , 62-75.		19
32	Exploring the Evolution of Novel Enzyme Functions within Structurally Defined Protein Superfamilies. <i>PLoS Computational Biology</i> , 2012, 8, e1002403.	3.2	80
33	FunTree: a resource for exploring the functional evolution of structurally defined enzyme superfamilies. <i>Nucleic Acids Research</i> , 2012, 40, D776-D782.	14.5	44
34	New functional families (FunFams) in CATH to improve the mapping of conserved functional sites to 3D structures. <i>Nucleic Acids Research</i> , 2012, 41, D490-D498.	14.5	188
35	Current challenges in genome annotation through structural biology and bioinformatics. <i>Current Opinion in Structural Biology</i> , 2012, 22, 594-601.	5.7	14
36	Extending CATH: increasing coverage of the protein structure universe and linking structure with function. <i>Nucleic Acids Research</i> , 2011, 39, D420-D426.	14.5	126

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37	Model-building strategies for low-resolution X-ray crystallographic data. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2009, 65, 121-127.	2.5	19
38	Missing in action: enzyme functional annotations in biological databases. <i>Nature Chemical Biology</i> , 2009, 5, 521-525.	8.0	53
39	Comparative modelling by restraint-based conformational sampling. <i>BMC Structural Biology</i> , 2008, 8, 7.	2.3	8
40	Structural basis for inhibition of homologous recombination by the RecX protein. <i>EMBO Journal</i> , 2008, 27, 2259-2269.	7.8	41
41	Assembly and Channel Opening in a Bacterial Drug Efflux Machine. <i>Molecular Cell</i> , 2008, 30, 114-121.	9.7	155
42	Structure and Mechanism of Drug Efflux Machinery in Gram Negative Bacteria. <i>Current Drug Targets</i> , 2008, 9, 719-728.	2.1	28
43	Structure of an Xrcc4-DNA ligase IV yeast ortholog complex reveals a novel BRCT interaction mode. <i>DNA Repair</i> , 2006, 5, 362-368.	2.8	60
44	Is one solution good enough?. <i>Nature Structural and Molecular Biology</i> , 2006, 13, 184-185.	8.2	110
45	Conformer generation under restraints. <i>Current Opinion in Structural Biology</i> , 2006, 16, 160-165.	5.7	24
46	Knowledge-Based Real-Space Explorations for Low-Resolution Structure Determination. <i>Structure</i> , 2006, 14, 1313-1320.	3.3	27