Shaun M Kandathil

List of Publications by Year
in descending order

18 papers	1,635 citations	758635 12 h-index	996533 15 g-index
21 all docs	21 docs citations	21 times ranked	1469 citing authors

#	Article	IF	Citations
1	A guide to machine learning for biologists. Nature Reviews Molecular Cell Biology, 2022, 23, 40-55.	16.1	626
2	Ultrafast end-to-end protein structure prediction enables high-throughput exploration of uncharacterized proteins. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	26
3	Prediction of interresidue contacts with DeepMetaPSICOV in CASP13. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1092-1099.	1.5	102
4	Reliable Generation of Native-Like Decoys Limits Predictive Ability in Fragment-Based Protein Structure Prediction. Biomolecules, 2019, 9, 612.	1.8	0
5	Recent developments in deep learning applied to protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1179-1189.	1.5	56
6	Deep learning extends de novo protein modelling coverage of genomes using iteratively predicted structural constraints. Nature Communications, 2019, 10, 3977.	5.8	144
7	Uncommon mutational profiles of metastatic colorectal cancer detected during routine genotyping using next generation sequencing. Scientific Reports, 2019, 9, 7083.	1.6	5
8	High precision in protein contact prediction using fully convolutional neural networks and minimal sequence features. Bioinformatics, 2018, 34, 3308-3315.	1.8	157
9	Improved fragment-based protein structure prediction by redesign of search heuristics. Scientific Reports, 2018, 8, 13694.	1.6	12
10	On heuristic bias in fragment-assembly methods for protein structure prediction. , 2017, , .		0
11	Toward a detailed understanding of search trajectories in fragment assembly approaches to protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2016, 84, 411-426.	1.5	18
12	Generating, Maintaining, and Exploiting Diversity in a Memetic Algorithm for Protein Structure Prediction. Evolutionary Computation, 2016, 24, 577-607.	2.3	38
13	Using Machine Learning to Explore the Relevance of Local and Global Features During Conformational Search in Rosetta. , 2015, , .		1
14	Accurate prediction of polarised high order electrostatic interactions for hydrogen bonded complexes using the machine learning method kriging. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 32-41.	2.0	19
15	The prediction of atomic kinetic energies from coordinates of surrounding atoms using kriging machine learning. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	20
16	Proton tunnelling and promoting vibrations during the oxidation of ascorbate by ferricyanide?. Physical Chemistry Chemical Physics, 2014, 16, 2256.	1.3	10
17	Accuracy and tractability of a kriging model of intramolecular polarizable multipolar electrostatics and its application to histidine. Journal of Computational Chemistry, 2013, 34, 1850-1861.	1.5	47
18	A review of the chemistry and pharmacology of the date fruits (Phoenix dactylifera L.). Food Research International, 2011, 44, 1812-1822.	2.9	320