

Vikram Khipple Mulligan

List of Publications by Year in descending order

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Version: 2024-02-01

32
papers

4,145
citations

304743

22
h-index

434195

31
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36
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docs citations

36
times ranked

5125
citing authors

#	ARTICLE	IF	CITATIONS
1	The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3031-3048.	5.3	1,032
2	Macromolecular modeling and design in Rosetta: recent methods and frameworks. <i>Nature Methods</i> , 2020, 17, 665-680.	19.0	513
3	Global analysis of protein folding using massively parallel design, synthesis, and testing. <i>Science</i> , 2017, 357, 168-175.	12.6	392
4	Simultaneous Optimization of Biomolecular Energy Functions on Features from Small Molecules and Macromolecules. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 6201-6212.	5.3	382
5	Accurate de novo design of hyperstable constrained peptides. <i>Nature</i> , 2016, 538, 329-335.	27.8	327
6	De novo design of bioactive protein switches. <i>Nature</i> , 2019, 572, 205-210.	27.8	190
7	Accurate computational design of multipass transmembrane proteins. <i>Science</i> , 2018, 359, 1042-1046.	12.6	149
8	Comprehensive computational design of ordered peptide macrocycles. <i>Science</i> , 2017, 358, 1461-1466.	12.6	146
9	Programmable design of orthogonal protein heterodimers. <i>Nature</i> , 2019, 565, 106-111.	27.8	139
10	Prion disease susceptibility is affected by β^2 -structure folding propensity and local side-chain interactions in PrP. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 19808-19813.	7.1	119
11	Computational Design of an Unnatural Amino Acid Dependent Metalloprotein with Atomic Level Accuracy. <i>Journal of the American Chemical Society</i> , 2013, 135, 13393-13399.	13.7	95
12	<i>Drosophila melanogaster</i> Cad99C, the orthologue of human Usher cadherin PCDH15, regulates the length of microvilli. <i>Journal of Cell Biology</i> , 2005, 171, 549-558.	5.2	72
13	Protein misfolding in the late-onset neurodegenerative diseases: Common themes and the unique case of amyotrophic lateral sclerosis. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013, 81, 1285-1303.	2.6	69
14	CCM3/PDCD10 Heterodimerizes with Germinal Center Kinase III (GCKIII) Proteins Using a Mechanism Analogous to CCM3 Homodimerization. <i>Journal of Biological Chemistry</i> , 2011, 286, 25056-25064.	3.4	67
15	De novo design of covalently constrained mesosize protein scaffolds with unique tertiary structures. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 10852-10857.	7.1	52
16	Denaturational Stress Induces Formation of Zinc-Deficient Monomers of Cu,Zn Superoxide Dismutase: Implications for Pathogenesis in Amyotrophic Lateral Sclerosis. <i>Journal of Molecular Biology</i> , 2008, 383, 424-436.	4.2	44
17	Early Steps in Oxidation-Induced SOD1 Misfolding: Implications for Non-Amyloid Protein Aggregation in Familial ALS. <i>Journal of Molecular Biology</i> , 2012, 421, 631-652.	4.2	44
18	Computationally designed peptide macrocycle inhibitors of New Delhi metallo- β -lactamase 1. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	41

#	ARTICLE	IF	CITATIONS
19	ALS-Causing SOD1 Mutations Promote Production of Copper-Deficient Misfolded Species. <i>Journal of Molecular Biology</i> , 2011, 409, 839-852.	4.2	39
20	Anchor extension: a structure-guided approach to design cyclic peptides targeting enzyme active sites. <i>Nature Communications</i> , 2021, 12, 3384.	12.8	37
21	The emerging role of computational design in peptide macrocycle drug discovery. <i>Expert Opinion on Drug Discovery</i> , 2020, 15, 833-852.	5.0	27
22	Better together: Elements of successful scientific software development in a distributed collaborative community. <i>PLoS Computational Biology</i> , 2020, 16, e1007507.	3.2	27
23	A systematic study of minima in alanine dipeptide. <i>Journal of Computational Chemistry</i> , 2019, 40, 297-309.	3.3	25
24	Computational design of mixed chirality peptide macrocycles with internal symmetry. <i>Protein Science</i> , 2020, 29, 2433-2445.	7.6	16
25	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. <i>Nature Communications</i> , 2021, 12, 6947.	12.8	16
26	MHCEpitopeEnergy, a Flexible Rosetta-Based Biotherapeutic Deimmunization Platform. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2368-2382.	5.4	12
27	Conversion of A β 42 into a Folded Soluble Native-like Protein using a Semi-random Library of Amphipathic Helices. <i>Journal of Molecular Biology</i> , 2010, 396, 1284-1294.	4.2	10
28	Current directions in combining simulation-based macromolecular modeling approaches with deep learning. <i>Expert Opinion on Drug Discovery</i> , 2021, 16, 1025-1044.	5.0	8
29	XENet: Using a new graph convolution to accelerate the timeline for protein design on quantum computers. <i>PLoS Computational Biology</i> , 2021, 17, e1009037.	3.2	8
30	Analyzing complicated protein folding kinetics rapidly by analytical Laplace inversion using a Tikhonov regularization variant. <i>Analytical Biochemistry</i> , 2012, 421, 181-190.	2.4	7
31	A computational method for the design of nested proteins by loop-directed domain insertion. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 354-369.	2.6	1
32	Correction: <i>Drosophila melanogaster</i> Cad99C, the orthologue of human Usher cadherin PCDH15, regulates the length of microvilli. <i>Journal of Cell Biology</i> , 2005, 171, 1085-1085.	5.2	0