Vikram Khipple Mulligan

List of Publications by Year
in descending order

32 papers	4,145 citations	304743 22 h-index	434195 31 g-index
36 all docs	36 docs citations	36 times ranked	5125 citing authors

#	Article	IF	Citations
1	Computationally designed peptide macrocycle inhibitors of New Delhi metallo-Î²-lactamase 1. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	41
2	MHCEpitopeEnergy, a Flexible Rosetta-Based Biotherapeutic Deimmunization Platform. Journal of Chemical Information and Modeling, 2021, 61, 2368-2382.	5.4	12
3	Current directions in combining simulation-based macromolecular modeling approaches with deep learning. Expert Opinion on Drug Discovery, 2021, 16, 1025-1044.	5.0	8
4	Anchor extension: a structure-guided approach to design cyclic peptides targeting enzyme active sites. Nature Communications, 2021, 12, 3384.	12.8	37
5	XENet: Using a new graph convolution to accelerate the timeline for protein design on quantum computers. PLoS Computational Biology, 2021, 17, e1009037.	3.2	8
6	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Nature Communications, 2021, 12, 6947.	12.8	16
7	Computational design of mixed chirality peptide macrocycles with internal symmetry. Protein Science, 2020, 29, 2433-2445.	7.6	16
8	The emerging role of computational design in peptide macrocycle drug discovery. Expert Opinion on Drug Discovery, 2020, 15, 833-852.	5.0	27
9	Better together: Elements of successful scientific software development in a distributed collaborative community. PLoS Computational Biology, 2020, 16, e1007507.	3.2	27
10	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	19.0	513
11	De novo design of bioactive protein switches. Nature, 2019, 572, 205-210.	27.8	190
12	Programmable design of orthogonal protein heterodimers. Nature, 2019, 565, 106-111.	27.8	139
13	A systematic study of minima in alanine dipeptide. Journal of Computational Chemistry, 2019, 40, 297-309.	3.3	25
14	Accurate computational design of multipass transmembrane proteins. Science, 2018, 359, 1042-1046.	12.6	149
15	A computational method for the design of nested proteins by loopâ€directed domain insertion. Proteins: Structure, Function and Bioinformatics, 2018, 86, 354-369.	2.6	1
16	The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design. Journal of Chemical Theory and Computation, 2017, 13, 3031-3048.	5.3	1,032
17	De novo design of covalently constrained mesosize protein scaffolds with unique tertiary structures. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10852-10857.	7.1	52
18	Global analysis of protein folding using massively parallel design, synthesis, and testing. Science, 2017, 357, 168-175.	12.6	392

#	Article	IF	Citations
19	Comprehensive computational design of ordered peptide macrocycles. Science, 2017, 358, 1461-1466.	12.6	146
20	Accurate de novo design of hyperstable constrained peptides. Nature, 2016, 538, 329-335.	27.8	327
21	Simultaneous Optimization of Biomolecular Energy Functions on Features from Small Molecules and Macromolecules. Journal of Chemical Theory and Computation, 2016, 12, 6201-6212.	5.3	382
22	Computational Design of an Unnatural Amino Acid Dependent Metalloprotein with Atomic Level Accuracy. Journal of the American Chemical Society, 2013, 135, 13393-13399.	13.7	95
23	Protein misfolding in the lateâ€onset neurodegenerative diseases: Common themes and the unique case of amyotrophic lateral sclerosis. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1285-1303.	2.6	69
24	Early Steps in Oxidation-Induced SOD1 Misfolding: Implications for Non-Amyloid Protein Aggregation in Familial ALS. Journal of Molecular Biology, 2012, 421, 631-652.	4.2	44
25	Analyzing complicated protein folding kinetics rapidly by analytical Laplace inversion using a Tikhonov regularization variant. Analytical Biochemistry, 2012, 421, 181-190.	2.4	7
26	ALS-Causing SOD1 Mutations Promote Production of Copper-Deficient Misfolded Species. Journal of Molecular Biology, 2011, 409, 839-852.	4.2	39
27	CCM3/PDCD10 Heterodimerizes with Germinal Center Kinase III (GCKIII) Proteins Using a Mechanism Analogous to CCM3 Homodimerization. Journal of Biological Chemistry, 2011, 286, 25056-25064.	3.4	67
28	Prion disease susceptibility is affected by Î²-structure folding propensity and local side-chain interactions in PrP. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 19808-19813.	7.1	119
29	Conversion of AÎ²42 into a Folded Soluble Native-like Protein using a Semi-random Library of Amphipathic Helices. Journal of Molecular Biology, 2010, 396, 1284-1294.	4.2	10
30	Denaturational Stress Induces Formation of Zinc-Deficient Monomers of Cu,Zn Superoxide Dismutase: Implications for Pathogenesis in Amyotrophic Lateral Sclerosis. Journal of Molecular Biology, 2008, 383, 424-436.	4.2	44
31	Correction: Drosophila melanogaster Cad99C, the orthologue of human Usher cadherin PCDH15, regulates the length of microvilli. Journal of Cell Biology, 2005, 171, 1085-1085.	5.2	0
32	Drosophila melanogaster Cad99C, the orthologue of human Usher cadherin PCDH15, regulates the length of microvilli. Journal of Cell Biology, 2005, 171, 549-558.	5.2	72