Vikram Khipple Mulligan

List of Publications by Year in Descending Order

35 papers	2,431 citations	19 h-index	36 g-index
36 ext. papers	3,373 ext. citations	14 avg, IF	4.84 L-index

#	Paper	IF	Citations
35	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. *Nature Communications*, **2021**, 12, 6947	17.4	0
34	Computationally designed peptide macrocycle inhibitors of New Delhi metallo-β-lactamase 1. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	17
33	MHCEpitopeEnergy, a Flexible Rosetta-Based Biotherapeutic Deimmunization Platform. *Journal of Chemical Information and Modeling*, **2021**, 61, 2368-2382	6.1	6
32	Current directions in combining simulation-based macromolecular modeling approaches with deep learning. *Expert Opinion on Drug Discovery*, **2021**, 16, 1025-1044	6.2	3
31	Anchor extension: a structure-guided approach to design cyclic peptides targeting enzyme active sites. *Nature Communications*, **2021**, 12, 3384	17.4	12
30	XENet: Using a new graph convolution to accelerate the timeline for protein design on quantum computers. *PLoS Computational Biology*, **2021**, 17, e1009037	5	2
29	The emerging role of computational design in peptide macrocycle drug discovery. *Expert Opinion on Drug Discovery*, **2020**, 15, 833-852	6.2	15
28	Better together: Elements of successful scientific software development in a distributed collaborative community. *PLoS Computational Biology*, **2020**, 16, e1007507	5	15
27	Macromolecular modeling and design in Rosetta: recent methods and frameworks. *Nature Methods*, **2020**, 17, 665-680	21.6	165
26	Computational design of mixed chirality peptide macrocycles with internal symmetry. *Protein Science*, **2020**, 29, 2433-2445	6.3	9
25	De novo design of bioactive protein switches. *Nature*, **2019**, 572, 205-210	50.4	113
24	Programmable design of orthogonal protein heterodimers. *Nature*, **2019**, 565, 106-111	50.4	87
23	A systematic study of minima in alanine dipeptide. *Journal of Computational Chemistry*, **2019**, 40, 297-309	3.5	15
22	Accurate computational design of multipass transmembrane proteins. *Science*, **2018**, 359, 1042-1046	33.3	93
21	A computational method for the design of nested proteins by loop-directed domain insertion. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86, 354-369	4.2	1
20	The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design. *Journal of Chemical Theory and Computation*, **2017**, 13, 3031-3048	6.4	486
19	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	11.5	44

18	Global analysis of protein folding using massively parallel design, synthesis, and testing. *Science*, **2017**, 357, 168-175	33.3	241
17	Comprehensive computational design of ordered peptide macrocycles. *Science*, **2017**, 358, 1461-1466	33.3	96
16	Accurate de novo design of hyperstable constrained peptides. *Nature*, **2016**, 538, 329-335	50.4	231
15	Simultaneous Optimization of Biomolecular Energy Functions on Features from Small Molecules and Macromolecules. *Journal of Chemical Theory and Computation*, **2016**, 12, 6201-6212	6.4	199
14	Computational design of an unnatural amino acid dependent metalloprotein with atomic level accuracy. *Journal of the American Chemical Society*, **2013**, 135, 13393-9	16.4	84
13	Protein misfolding in the late-onset neurodegenerative diseases: common themes and the unique case of amyotrophic lateral sclerosis. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 1285-303	4.2	62
12	Early steps in oxidation-induced SOD1 misfolding: implications for non-amyloid protein aggregation in familial ALS. *Journal of Molecular Biology*, **2012**, 421, 631-52	6.5	38
11	Analyzing complicated protein folding kinetics rapidly by analytical Laplace inversion using a Tikhonov regularization variant. *Analytical Biochemistry*, **2012**, 421, 181-90	3.1	7
10	ALS-causing SOD1 mutations promote production of copper-deficient misfolded species. *Journal of Molecular Biology*, **2011**, 409, 839-52	6.5	33
9	CCM3/PDCD10 heterodimerizes with germinal center kinase III (GCKIII) proteins using a mechanism analogous to CCM3 homodimerization. *Journal of Biological Chemistry*, **2011**, 286, 25056-64	5.4	50
8	Prion disease susceptibility is affected by beta-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, 19808-13	11.5	102
7	Conversion of Abeta42 into a folded soluble native-like protein using a semi-random library of amphipathic helices. *Journal of Molecular Biology*, **2010**, 396, 1284-94	6.5	10
6	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, 424-36	6.5	40
5	Correction: Drosophila melanogaster Cad99C, the orthologue of human Usher cadherin PCDH15, regulates the length of microvilli. *Journal of Cell Biology*, **2005**, 171, 1085-1085	7.3	78
4	Drosophila melanogaster Cad99C, the orthologue of human Usher cadherin PCDH15, regulates the length of microvilli. *Journal of Cell Biology*, **2005**, 171, 549-58	7.3	59
3	The Rosetta all-atom energy function for macromolecular modeling and design		3
2	Designing Peptides on a Quantum Computer		13
1	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks		2