John Karanicolas

List of Publications by Citations

60 papers	5,075 citations	27 h-index	67 g-index
67 ext. papers	6,180 ext. citations	8.6 avg, IF	5.53 L-index

#	Paper	IF	Citations
60	ROSETTA3: an object-oriented software suite for the simulation and design of macromolecules. *Methods in Enzymology*, **2011**, 487, 545-74	1.7	1216
59	MMTSB Tool Set: enhanced sampling and multiscale modeling methods for applications in structural biology. *Journal of Molecular Graphics and Modelling*, **2004**, 22, 377-95	2.8	709
58	Structure-based design of non-natural amino-acid inhibitors of amyloid fibril formation. *Nature*, **2011**, 475, 96-100	50.4	341
57	The 3D profile method for identifying fibril-forming segments of proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 4074-8	11.5	325
56	The origins of asymmetry in the folding transition states of protein L and protein G. *Protein Science*, **2002**, 11, 2351-61	6.3	313
55	Atomic accuracy in predicting and designing noncanonical RNA structure. *Nature Methods*, **2010**, 7, 291-4	21.6	263
54	Improved Gō-like models demonstrate the robustness of protein folding mechanisms towards non-native interactions. *Journal of Molecular Biology*, **2003**, 334, 309-25	6.5	175
53	Macromolecular modeling and design in Rosetta: recent methods and frameworks. *Nature Methods*, **2020**, 17, 665-680	21.6	165
52	Allostery in Its Many Disguises: From Theory to Applications. *Structure*, **2019**, 27, 566-578	5.2	158
51	A de novo protein binding pair by computational design and directed evolution. *Molecular Cell*, **2011**, 42, 250-60	17.6	141
50	The structural basis for biphasic kinetics in the folding of the WW domain from a formin-binding protein: lessons for protein design?. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 3954-9	11.5	119
49	Musashi RNA-Binding Proteins as Cancer Drivers and Novel Therapeutic Targets. *Clinical Cancer Research*, **2017**, 23, 2143-2153	12.9	115
48	Targeting CDK9 Reactivates Epigenetically Silenced Genes in Cancer. *Cell*, **2018**, 175, 1244-1258.e26	56.2	102
47	Natural product (-)-gossypol inhibits colon cancer cell growth by targeting RNA-binding protein Musashi-1. *Molecular Oncology*, **2015**, 9, 1406-20	7.9	82
46	Druggable protein interaction sites are more predisposed to surface pocket formation than the rest of the protein surface. *PLoS Computational Biology*, **2013**, 9, e1002951	5	64
45	Integrating folding kinetics and protein function: biphasic kinetics and dual binding specificity in a WW domain. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 3432-7	11.5	61
44	Site-specific incorporation of photoisomerizable azobenzene groups into ribonuclease S. *Bioorganic and Medicinal Chemistry Letters*, **1997**, 7, 2677-2680	2.9	54

43	Isothermal Analysis of ThermoFluor Data can readily provide Quantitative Binding Affinities. *Scientific Reports*, **2019**, 9, 2650	4.9	47
42	Machine learning classification can reduce false positives in structure-based virtual screening. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 18477-18488	11.5	47
41	Promysalin Elicits Species-Selective Inhibition of Pseudomonas aeruginosa by Targeting Succinate Dehydrogenase. *Journal of the American Chemical Society*, **2018**, 140, 1774-1782	16.4	46
40	Designing allosteric control into enzymes by chemical rescue of structure. *Journal of the American Chemical Society*, **2012**, 134, 10055-60	16.4	33
39	Ultra-High-Throughput Structure-Based Virtual Screening for Small-Molecule Inhibitors of Protein-Protein Interactions. *Journal of Chemical Information and Modeling*, **2016**, 56, 399-411	6.1	32
38	Hotspot-centric de novo design of protein binders. *Journal of Molecular Biology*, **2011**, 413, 1047-62	6.5	32
37	Rationally designed integrin beta3 mutants stabilized in the high affinity conformation. *Journal of Biological Chemistry*, **2009**, 284, 3917-24	5.4	32
36	The importance of explicit chain representation in protein folding models: an examination of Ising-like models. *Proteins: Structure, Function and Bioinformatics*, **2003**, 53, 740-7	4.2	30
35	Optogenetic Inhibitor of the Transcription Factor CREB. *Chemistry and Biology*, **2015**, 22, 1531-1539		29
34	The fungal natural product azaphilone-9 binds to HuR and inhibits HuR-RNA interaction in vitro. *PLoS ONE*, **2017**, 12, e0175471	3.7	28
33	When Does Chemical Elaboration Induce a Ligand To Change Its Binding Mode?. *Journal of Medicinal Chemistry*, **2017**, 60, 128-145	8.3	27
32	Targeting the interaction between RNA-binding protein HuR and FOXQ1 suppresses breast cancer invasion and metastasis. *Communications Biology*, **2020**, 3, 193	6.7	24
31	Structural properties of non-traditional drug targets present new challenges for virtual screening. *Journal of Chemical Information and Modeling*, **2013**, 53, 2073-81	6.1	23
30	Rationalizing PROTAC-Mediated Ternary Complex Formation Using Rosetta. *Journal of Chemical Information and Modeling*, **2021**, 61, 1368-1382	6.1	22
29	The designability of protein switches by chemical rescue of structure: mechanisms of inactivation and reactivation. *Journal of the American Chemical Society*, **2013**, 135, 18840-9	16.4	21
28	Natural product derivative Gossypolone inhibits Musashi family of RNA-binding proteins. *BMC Cancer*, **2018**, 18, 809	4.8	18
27	Selectivity by small-molecule inhibitors of protein interactions can be driven by protein surface fluctuations. *PLoS Computational Biology*, **2015**, 11, e1004081	5	17
26	DARC: Mapping Surface Topography by Ray-Casting for Effective Virtual Screening at Protein Interaction Sites. *Journal of Medicinal Chemistry*, **2016**, 59, 4152-70	8.3	16

25	Enhancements to the Rosetta Energy Function Enable Improved Identification of Small Molecules that Inhibit Protein-Protein Interactions. *PLoS ONE*, **2015**, 10, e0140359	3.7	16
24	Impact of antibiotic treatment and host innate immune pressure on enterococcal adaptation in the human bloodstream. *Science Translational Medicine*, **2019**, 11,	17.5	13
23	Effect of single-point mutations on the stability and immunogenicity of a recombinant ricin A chain subunit vaccine antigen. *Human Vaccines and Immunotherapeutics*, **2013**, 9, 744-52	4.4	12
22	DARC 2.0: Improved Docking and Virtual Screening at Protein Interaction Sites. *PLoS ONE*, **2015**, 10, e0131612	3.7	12
21	Identification of novel small molecule Beclin 1 mimetics activating autophagy. *Oncotarget*, **2017**, 8, 51355-51369	5.5	12
20	Using homology modeling to interrogate binding affinity in neutralization of ricin toxin by a family of single domain antibodies. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 1994-2008	4.2	11
19	Fast docking on graphics processing units via Ray-Casting. *PLoS ONE*, **2013**, 8, e70661	3.7	8
18	Novel Ricin Subunit Antigens With Enhanced Capacity to Elicit Toxin-Neutralizing Antibody Responses in Mice. *Journal of Pharmaceutical Sciences*, **2016**, 105, 1603-1613	3.9	7
17	Full and Partial Agonism of a Designed Enzyme Switch. *ACS Synthetic Biology*, **2016**, 5, 1475-1484	5.7	7
16	Computational Screening and Design for Compounds that Disrupt Protein-protein Interactions. *Current Topics in Medicinal Chemistry*, **2017**, 17, 2703-2714	3	6
15	Leveraging a Low-Affinity Diazaspiro Orthosteric Fragment to Reduce Dopamine D Receptor (DR) Ligand Promiscuity across Highly Conserved Aminergic G-Protein-Coupled Receptors (GPCRs). *Journal of Medicinal Chemistry*, **2019**, 62, 5132-5147	8.3	5
14	Rationalizing PROTAC-mediated ternary complex formation using Rosetta		5
13	Chaperonin-Based Biolayer Interferometry To Assess the Kinetic Stability of Metastable, Aggregation-Prone Proteins. *Biochemistry*, **2016**, 55, 4885-908	3.2	5
12	A clinically relevant polymorphism in the Na/taurocholate cotransporting polypeptide (NTCP) occurs at a rheostat position. *Journal of Biological Chemistry*, **2021**, 296, 100047	5.4	4
11	"Solvent hydrogen-bond occlusion": A new model of polar desolvation for biomolecular energetics. *Journal of Computational Chemistry*, **2017**, 38, 1321-1331	3.5	3
10	Computational Design of an Allosteric Antibody Switch by Deletion and Rescue of a Complex Structural Constellation. *ACS Central Science*, **2020**, 6, 390-403	16.8	3
9	Identification and Validation of an Secondary Metabolite Derivative as an Inhibitor of the Musashi-RNA Interaction. *Cancers*, **2020**, 12,	6.6	3
8	Target-Based Design of Promysalin Analogues Identifies a New Putative Binding Cleft in Succinate Dehydrogenase. *ACS Infectious Diseases*, **2020**, 6, 1372-1377	5.5	2

List of Publications

7	Modulating Antibody Structure and Function through Directed Mutations and Chemical Rescue. *ACS Synthetic Biology*, **2018**, 7, 1152-1162	5.7	2
6	Designing orthogonal signaling pathways: how to fit in with the surroundings. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 5140-1	11.5	2
5	Comparative Modeling of CDK9 Inhibitors to Explore Selectivity and Structure-Activity Relationships		2
4	Contribution of an unusual CDR2 element of a single domain antibody in ricin toxin binding affinity and neutralizing activity. *Protein Engineering, Design and Selection*, **2018**, 31, 277-287	1.9	2
3	Optimal allosteric stabilization sites using contact stabilization analysis. *Journal of Computational Chemistry*, **2017**, 38, 1138-1146	3.5	1
2	Integrative genome-wide analysis reveals EIF3A as a key downstream regulator of translational repressor protein Musashi 2 (MSI2).. *NAR Cancer*, **2022**, 4, zcac015	5.2	0
1	An evolution of minimalist models for protein folding: from the behavior of protein-like polymers to protein function. *Drug Discovery Today Biosilico*, **2004**, 2, 127-133		