Tanja Kortemme

List of Publications by Citations

93 papers	12,087 citations	46 h-index	105 g-index
105 ext. papers	15,249 ext. citations	11.5 avg, IF	6.22 L-index

#	Paper	IF	Citations
93	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. *Nature*, **2020**, 583, 459-468	50.4	2142
92	ROSETTA3: an object-oriented software suite for the simulation and design of macromolecules. *Methods in Enzymology*, **2011**, 487, 545-74	1.7	1216
91	A simple physical model for binding energy hot spots in protein-protein complexes. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 14116-21	11.5	656
90	Global landscape of HIV-human protein complexes. *Nature*, **2011**, 481, 365-70	50.4	507
89	The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design. *Journal of Chemical Theory and Computation*, **2017**, 13, 3031-3048	6.4	486
88	The Global Phosphorylation Landscape of SARS-CoV-2 Infection. *Cell*, **2020**, 182, 685-712.e19	56.2	439
87	An orientation-dependent hydrogen bonding potential improves prediction of specificity and structure for proteins and protein-protein complexes. *Journal of Molecular Biology*, **2003**, 326, 1239-59	6.5	429
86	Ca2+ indicators based on computationally redesigned calmodulin-peptide pairs. *Chemistry and Biology*, **2006**, 13, 521-30		402
85	Computational alanine scanning of protein-protein interfaces. *Science Signaling*, **2004**, 2004, pl2	8.8	361
84	Sub-angstrom accuracy in protein loop reconstruction by robotics-inspired conformational sampling. *Nature Methods*, **2009**, 6, 551-2	21.6	329
83	Comparative host-coronavirus protein interaction networks reveal pan-viral disease mechanisms. *Science*, **2020**, 370,	33.3	261
82	Computational redesign of protein-protein interaction specificity. *Nature Structural and Molecular Biology*, **2004**, 11, 371-9	17.6	254
81	Backrub-like backbone simulation recapitulates natural protein conformational variability and improves mutant side-chain prediction. *Journal of Molecular Biology*, **2008**, 380, 742-56	6.5	232
80	Serverification of molecular modeling applications: the Rosetta Online Server that Includes Everyone (ROSIE). *PLoS ONE*, **2013**, 8, e63906	3.7	230
79	Close agreement between the orientation dependence of hydrogen bonds observed in protein structures and quantum mechanical calculations. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 6946-51	11.5	211
78	Design, activity, and structure of a highly specific artificial endonuclease. *Molecular Cell*, **2002**, 10, 895-905	17.6	202
77	SNX27 mediates PDZ-directed sorting from endosomes to the plasma membrane. *Journal of Cell Biology*, **2010**, 190, 565-74	7.3	193

76	Computational design of protein-protein interactions. *Current Opinion in Chemical Biology*, **2004**, 8, 91-7	9.7	187
75	Macromolecular modeling and design in Rosetta: recent methods and frameworks. *Nature Methods*, **2020**, 17, 665-680	21.6	165
74	Scientific benchmarks for guiding macromolecular energy function improvement. *Methods in Enzymology*, **2013**, 523, 109-43	1.7	164
73	Combined covalent-electrostatic model of hydrogen bonding improves structure prediction with Rosetta. *Journal of Chemical Theory and Computation*, **2015**, 11, 609-22	6.4	163
72	A SARS-CoV-2-Human Protein-Protein Interaction Map Reveals Drug Targets and Potential Drug-Repurposing **2020**,		133
71	Computer-aided design of functional protein interactions. *Nature Chemical Biology*, **2009**, 5, 797-807	11.7	131
70	The design of linear peptides that fold as monomeric beta-sheet structures. *Current Opinion in Structural Biology*, **1999**, 9, 487-93	8.1	122
69	Computational design of a new hydrogen bond network and at least a 300-fold specificity switch at a protein-protein interface. *Journal of Molecular Biology*, **2006**, 361, 195-208	6.5	119
68	Improvements to robotics-inspired conformational sampling in rosetta. *PLoS ONE*, **2013**, 8, e63090	3.7	115
67	Engineered ACE2 receptor traps potently neutralize SARS-CoV-2. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 28046-28055	11.5	110
66	Convergent mechanisms for recognition of divergent cytokines by the shared signaling receptor gp130. *Molecular Cell*, **2003**, 12, 577-89	17.6	107
65	RosettaBackrub--a web server for flexible backbone protein structure modeling and design. *Nucleic Acids Research*, **2010**, 38, W569-75	20.1	94
64	Symmetry recognizing asymmetry: analysis of the interactions between the C-type lectin-like immunoreceptor NKG2D and MHC class I-like ligands. *Structure*, **2003**, 11, 411-22	5.2	90
63	Design of multi-specificity in protein interfaces. *PLoS Computational Biology*, **2007**, 3, e164	5	87
62	Structure-based prediction of the peptide sequence space recognized by natural and synthetic PDZ domains. *Journal of Molecular Biology*, **2010**, 402, 460-74	6.5	84
61	Backbone flexibility in computational protein design. *Current Opinion in Biotechnology*, **2009**, 20, 420-8	11.4	84
60	Controlling CRISPR-Cas9 with ligand-activated and ligand-deactivated sgRNAs. *Nature Communications*, **2019**, 10, 2127	17.4	82
59	Flex ddG: Rosetta Ensemble-Based Estimation of Changes in Protein-Protein Binding Affinity upon Mutation. *Journal of Physical Chemistry B*, **2018**, 122, 5389-5399	3.4	80

58	Cost-benefit tradeoffs in engineered lac operons. *Science*, **2012**, 336, 911-5	33.3	74
57	Predicting the tolerated sequences for proteins and protein interfaces using RosettaBackrub flexible backbone design. *PLoS ONE*, **2011**, 6, e20451	3.7	73
56	Prediction of protein-protein interface sequence diversity using flexible backbone computational protein design. *Structure*, **2008**, 16, 1777-88	5.2	69
55	Control of protein signaling using a computationally designed GTPase/GEF orthogonal pair. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 5277-82	11.5	67
54	A new hydrogen-bonding potential for the design of protein-RNA interactions predicts specific contacts and discriminates decoys. *Nucleic Acids Research*, **2004**, 32, 5147-62	20.1	62
53	A correspondence between solution-state dynamics of an individual protein and the sequence and conformational diversity of its family. *PLoS Computational Biology*, **2009**, 5, e1000393	5	60
52	A simple model of backbone flexibility improves modeling of side-chain conformational variability. *Journal of Molecular Biology*, **2008**, 380, 757-74	6.5	60
51	Deconstruction of the Ras switching cycle through saturation mutagenesis. *ELife*, **2017**, 6,	8.9	58
50	A Web Resource for Standardized Benchmark Datasets, Metrics, and Rosetta Protocols for Macromolecular Modeling and Design. *PLoS ONE*, **2015**, 10, e0130433	3.7	58
49	Rational design of intercellular adhesion molecule-1 (ICAM-1) variants for antagonizing integrin lymphocyte function-associated antigen-1-dependent adhesion. *Journal of Biological Chemistry*, **2006**, 281, 5042-9	5.4	49
48	Evaluation of Models of Electrostatic Interactions in Proteins. *Journal of Physical Chemistry B*, **2003**, 107, 2075-2090	3.4	46
47	Coupling Protein Side-Chain and Backbone Flexibility Improves the Re-design of Protein-Ligand Specificity. *PLoS Computational Biology*, **2015**, 11, e1004335	5	46
46	Multi-constraint computational design suggests that native sequences of germline antibody H3 loops are nearly optimal for conformational flexibility. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 846-58	4.2	45
45	Reprogramming an ATP-driven protein machine into a light-gated nanocage. *Nature Nanotechnology*, **2013**, 8, 928-32	28.7	44
44	Determination of ubiquitin fitness landscapes under different chemical stresses in a classroom setting. *ELife*, **2016**, 5,	8.9	44
43	Potential functions for hydrogen bonds in protein structure prediction and design. *Advances in Protein Chemistry*, **2005**, 72, 1-38		38
42	Flexible backbone sampling methods to model and design protein alternative conformations. *Methods in Enzymology*, **2013**, 523, 61-85	1.7	36
41	Computational design of a modular protein sense-response system. *Science*, **2019**, 366, 1024-1028	33.3	36

40	Engineering a light-activated caspase-3 for precise ablation of neurons in vivo. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E8174-E8183	11.5	32
39	Quantitative mapping of protein-peptide affinity landscapes using spectrally encoded beads. *ELife*, **2019**, 8,	8.9	29
38	Recent advances in de novo protein design: Principles, methods, and applications. *Journal of Biological Chemistry*, **2021**, 296, 100558	5.4	29
37	Expanding the space of protein geometries by computational design of de novo fold families. *Science*, **2020**, 369, 1132-1136	33.3	28
36	Assessment of flexible backbone protein design methods for sequence library prediction in the therapeutic antibody Herceptin-HER2 interface. *Protein Science*, **2011**, 20, 1082-9	6.3	27
35	Computational protein design quantifies structural constraints on amino acid covariation. *PLoS Computational Biology*, **2013**, 9, e1003313	5	25
34	Mutations designed to destabilize the receptor-bound conformation increase MICA-NKG2D association rate and affinity. *Journal of Biological Chemistry*, **2007**, 282, 30658-66	5.4	23
33	Designing ensembles in conformational and sequence space to characterize and engineer proteins. *Current Opinion in Structural Biology*, **2010**, 20, 377-84	8.1	22
32	A new twist in TCR diversity revealed by a forbidden alphabeta TCR. *Journal of Molecular Biology*, **2008**, 375, 1306-19	6.5	21
31	Design of a photoswitchable cadherin. *Journal of the American Chemical Society*, **2013**, 135, 12516-9	16.4	20
30	Comparison of Rosetta flexible-backbone computational protein design methods on binding interactions. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 206-226	4.2	20
29	Prediction of mutational tolerance in HIV-1 protease and reverse transcriptase using flexible backbone protein design. *PLoS Computational Biology*, **2012**, 8, e1002639	5	17
28	Computational design of structured loops for new protein functions. *Biological Chemistry*, **2019**, 400, 275-288	4.5	16
27	Quantification of the transferability of a designed protein specificity switch reveals extensive epistasis in molecular recognition. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 15426-31	11.5	16
26	Better together: Elements of successful scientific software development in a distributed collaborative community. *PLoS Computational Biology*, **2020**, 16, e1007507	5	15
25	Design of a phosphorylatable PDZ domain with peptide-specific affinity changes. *Structure*, **2013**, 21, 54-64	5.2	14
24	Amino-acid site variability among natural and designed proteins. *PeerJ*, **2013**, 1, e211	3.1	13
23	Extending chemical perturbations of the ubiquitin fitness landscape in a classroom setting reveals new constraints on sequence tolerance. *Biology Open*, **2018**, 7,	2.2	11

22	CryoEM and AI reveal a structure of SARS-CoV-2 Nsp2, a multifunctional protein involved in key host processes **2021**,		10
21	Engineered ACE2 receptor traps potently neutralize SARS-CoV-2 **2020**,		9
20	New computational protein design methods for de novo small molecule binding sites. *PLoS Computational Biology*, **2020**, 16, e1008178	5	9
19	Altered expression of a quality control protease in reshapes the in vivo mutational landscape of a model enzyme. *ELife*, **2020**, 9,	8.9	8
18	A Model for the Molecular Mechanism of an Engineered Light-Driven Protein Machine. *Structure*, **2016**, 24, 576-584	5.2	6
17	In support of the BMRB. *Nature Structural and Molecular Biology*, **2012**, 19, 854-60	17.6	5
16	CryoEM and AI reveal a structure of SARS-CoV-2 Nsp2, a multifunctional protein involved in key host processes **2021**,		4
15	Design principles of protein switches. *Current Opinion in Structural Biology*, **2021**, 72, 71-78	8.1	4
14	The Rosetta all-atom energy function for macromolecular modeling and design		3
13	Quantitative mapping of protein-peptide affinity landscapes using spectrally encoded beads		3
12	Design of Light-Controlled Protein Conformations and Functions. *Methods in Molecular Biology*, **2016**, 1414, 197-211	1.4	3
11	Author response: Deconstruction of the Ras switching cycle through saturation mutagenesis **2017**,		2
10	Flex ddG: Rosetta ensemble-based estimation of changes in protein-protein binding affinity upon mutation		2
9	Modulating the cellular context broadly reshapes the mutational landscape of a model enzyme		2
8	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks		2
7	Advances in the Computational Design of Small-Molecule-Controlled Protein-Based Circuits for Synthetic Biology. *Proceedings of the IEEE*, **2022**, 1-16	14.3	2
6	De novo protein fold families expand the designable ligand binding site space. *PLoS Computational Biology*, **2021**, 17, e1009620	5	1
5	Systems-level effects of allosteric perturbations to a model molecular switch. *Nature*, **2021**, 599, 152-157	50.4	1

4	Reply to Liu et al.: Specific mutations matter in specificity and catalysis in ACE2. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	1
3	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. *Nature Communications*, **2021**, 12, 6947	17.4	0
2	Accurate positioning of functional residues with robotics-inspired computational protein design.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2115480119	11.5	0
1	Design of Multi-Specificity in Protein Interfaces. *PLoS Computational Biology*, **2005**, preprint, e164	5	