Tanja Kortemme

List of Publications by Year
in descending order

84 papers	17,479 citations	41344 49 h-index	58581 82 g-index
105 all docs	105 docs citations	105 times ranked	24398 citing authors

#	Article	IF	Citations
1	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. Nature, 2020, 583, 459-468.	27.8	3,542
2	Rosetta3. Methods in Enzymology, 2011, 487, 545-574.	1.0	1,620
3	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
4	The Global Phosphorylation Landscape of SARS-CoV-2 Infection. Cell, 2020, 182, 685-712.e19.	28.9	825
5	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, 14116-14121.	7.1	754
6	Global landscape of HIVâ€“human protein complexes. Nature, 2012, 481, 365-370.	27.8	651
7	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	19.0	513
8	Comparative host-coronavirus protein interaction networks reveal pan-viral disease mechanisms. Science, 2020, 370, .	12.6	508
9	Computational Alanine Scanning of Protein-Protein Interfaces. Science Signaling, 2004, 2004, pl2-pl2.	3.6	471
10	An Orientation-dependent Hydrogen Bonding Potential Improves Prediction of Specificity and Structure for Proteins and Proteinâ€“Protein Complexes. Journal of Molecular Biology, 2003, 326, 1239-1259.	4.2	460
11	Ca2+ Indicators Based on Computationally Redesigned Calmodulin-Peptide Pairs. Chemistry and Biology, 2006, 13, 521-530.	6.0	455
12	Sub-angstrom accuracy in protein loop reconstruction by robotics-inspired conformational sampling. Nature Methods, 2009, 6, 551-552.	19.0	408
13	Serverification of Molecular Modeling Applications: The Rosetta Online Server That Includes Everyone (ROSIE). PLoS ONE, 2013, 8, e63906.	2.5	348
14	Backrub-Like Backbone Simulation Recapitulates Natural Protein Conformational Variability and Improves Mutant Side-Chain Prediction. Journal of Molecular Biology, 2008, 380, 742-756.	4.2	283
15	Computational redesign of protein-protein interaction specificity. Nature Structural and Molecular Biology, 2004, 11, 371-379.	8.2	279
16	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, 6946-6951.	7.1	227
17	SNX27 mediates PDZ-directed sorting from endosomes to the plasma membrane. Journal of Cell Biology, 2010, 190, 565-574.	5.2	222
18	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.	7.1	219

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19	Design, Activity, and Structure of a Highly Specific Artificial Endonuclease. Molecular Cell, 2002, 10, 895-905.	9.7	218
20	Computational design of proteinâ€"protein interactions. Current Opinion in Chemical Biology, 2004, 8, 91-97.	6.1	213
21	Combined Covalent-Electrostatic Model of Hydrogen Bonding Improves Structure Prediction with Rosetta. Journal of Chemical Theory and Computation, 2015, 11, 609-622.	5.3	204
22	Scientific Benchmarks for Guiding Macromolecular Energy Function Improvement. Methods in Enzymology, 2013, 523, 109-143.	1.0	195
23	Flex ddG: Rosetta Ensemble-Based Estimation of Changes in Proteinâ€"Protein Binding Affinity upon Mutation. Journal of Physical Chemistry B, 2018, 122, 5389-5399.	2.6	192
24	Improvements to Robotics-Inspired Conformational Sampling in Rosetta. PLoS ONE, 2013, 8, e63090.	2.5	176
25	Computer-aided design of functional protein interactions. Nature Chemical Biology, 2009, 5, 797-807.	8.0	144
26	Controlling CRISPR-Cas9 with ligand-activated and ligand-deactivated sgRNAs. Nature Communications, 2019, 10, 2127.	12.8	133
27	Convergent Mechanisms for Recognition of Divergent Cytokines by the Shared Signaling Receptor gp130. Molecular Cell, 2003, 12, 577-589.	9.7	131
28	The design of linear peptides that fold as monomeric Î²-sheet structures. Current Opinion in Structural Biology, 1999, 9, 487-493.	5.7	128
29	Computational Design of a New Hydrogen Bond Network and at Least a 300-fold Specificity Switch at a Proteinâ^'Protein Interface. Journal of Molecular Biology, 2006, 361, 195-208.	4.2	126
30	Recent advances in de novo protein design: Principles, methods, and applications. Journal of Biological Chemistry, 2021, 296, 100558.	3.4	120
31	RosettaBackrub--a web server for flexible backbone protein structure modeling and design. Nucleic Acids Research, 2010, 38, W569-W575.	14.5	110
32	Symmetry Recognizing Asymmetry. Structure, 2003, 11, 411-422.	3.3	99
33	Design of Multi-Specificity in Protein Interfaces. PLoS Computational Biology, 2007, 3, e164.	3.2	95
34	Deconstruction of the Ras switching cycle through saturation mutagenesis. ELife, 2017, 6, .	6.0	95
35	Predicting the Tolerated Sequences for Proteins and Protein Interfaces Using RosettaBackrub Flexible Backbone Design. PLoS ONE, 2011, 6, e20451.	2.5	94
36	Backbone flexibility in computational protein design. Current Opinion in Biotechnology, 2009, 20, 420-428.	6.6	93

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37	Structure-Based Prediction of the Peptide Sequence Space Recognized by Natural and Synthetic PDZ Domains. Journal of Molecular Biology, 2010, 402, 460-474.	4.2	92
38	Computational design of a modular protein sense-response system. Science, 2019, 366, 1024-1028.	12.6	91
39	Cost-Benefit Tradeoffs in Engineered <i>lac</i> Operons. Science, 2012, 336, 911-915.	12.6	90
40	A Web Resource for Standardized Benchmark Datasets, Metrics, and Rosetta Protocols for Macromolecular Modeling and Design. PLoS ONE, 2015, 10, e0130433.	2.5	85
41	Prediction of Protein-Protein Interface Sequence Diversity Using Flexible Backbone Computational Protein Design. Structure, 2008, 16, 1777-1788.	3.3	73
42	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, 5277-5282.	7.1	73
43	Coupling Protein Side-Chain and Backbone Flexibility Improves the Re-design of Protein-Ligand Specificity. PLoS Computational Biology, 2015, 11, e1004335.	3.2	71
44	Determination of ubiquitin fitness landscapes under different chemical stresses in a classroom setting. ELife, 2016, 5, .	6.0	71
45	A Simple Model of Backbone Flexibility Improves Modeling of Side-chain Conformational Variability. Journal of Molecular Biology, 2008, 380, 757-774.	4.2	67
46	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.	3.2	66
47	A new hydrogen-bonding potential for the design of protein-RNA interactions predicts specific contacts and discriminates decoys. Nucleic Acids Research, 2004, 32, 5147-5162.	14.5	64
48	Potential Functions for Hydrogen Bonds in Protein Structure Prediction and Design. Advances in Protein Chemistry, 2005, 72, 1-38.	4.4	57
49	Expanding the space of protein geometries by computational design of de novo fold families. Science, 2020, 369, 1132-1136.	12.6	57
50	Multiâ€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, 846-858.	2.6	56
51	Reprogramming an ATP-driven protein machine into a light-gated nanocage. Nature Nanotechnology, 2013, 8, 928-932.	31.5	55
52	Quantitative mapping of protein-peptide affinity landscapes using spectrally encoded beads. ELife, 2019, 8, .	6.0	53
53	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, 5042-5049.	3.4	52
54	Evaluation of Models of Electrostatic Interactions in Proteins. Journal of Physical Chemistry B, 2003, 107, 2075-2090.	2.6	50

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55	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.	7.1	50
56	Flexible Backbone Sampling Methods to Model and Design Protein Alternative Conformations. Methods in Enzymology, 2013, 523, 61-85.	1.0	44
57	Altered expression of a quality control protease in E. coli reshapes the in vivo mutational landscape of a model enzyme. ELife, 2020, 9, .	6.0	37
58	Computational Protein Design Quantifies Structural Constraints on Amino Acid Covariation. PLoS Computational Biology, 2013, 9, e1003313.	3.2	35
59	Assessment of flexible backbone protein design methods for sequence library prediction in the therapeutic antibody Herceptinâ€"HER2 interface. Protein Science, 2011, 20, 1082-1089.	7.6	30
60	Comparison of Rosetta flexibleâ€backbone computational protein design methods on binding interactions. Proteins: Structure, Function and Bioinformatics, 2020, 88, 206-226.	2.6	27
61	Better together: Elements of successful scientific software development in a distributed collaborative community. PLoS Computational Biology, 2020, 16, e1007507.	3.2	27
62	Designing ensembles in conformational and sequence space to characterize and engineer proteins. Current Opinion in Structural Biology, 2010, 20, 377-384.	5.7	26
63	Mutations Designed to Destabilize the Receptor-Bound Conformation Increase MICA-NKG2D Association Rate and Affinity. Journal of Biological Chemistry, 2007, 282, 30658-30666.	3.4	25
64	Computational design of structured loops for new protein functions. Biological Chemistry, 2019, 400, 275-288.	2.5	25
65	Design of a Photoswitchable Cadherin. Journal of the American Chemical Society, 2013, 135, 12516-12519.	13.7	22
66	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, 15426-15431.	7.1	22
67	A New Twist in TCR Diversity Revealed by a Forbidden Î±Î² TCR. Journal of Molecular Biology, 2008, 375, 1306-1319.	4.2	21
68	Prediction of Mutational Tolerance in HIV-1 Protease and Reverse Transcriptase Using Flexible Backbone Protein Design. PLoS Computational Biology, 2012, 8, e1002639.	3.2	21
69	New computational protein design methods for de novo small molecule binding sites. PLoS Computational Biology, 2020, 16, e1008178.	3.2	20
70	Design principles of protein switches. Current Opinion in Structural Biology, 2022, 72, 71-78.	5.7	20
71	Amino-acid site variability among natural and designed proteins. PeerJ, 2013, 1, e211.	2.0	18
72	Design of a Phosphorylatable PDZ Domain with Peptide-Specific Affinity Changes. Structure, 2013, 21, 54-64.	3.3	17

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73	Extending chemical perturbations of the ubiquitin fitness landscape in a classroom setting reveals new constraints on sequence tolerance. Biology Open, 2018, 7, .	1.2	17
74	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Nature Communications, 2021, 12, 6947.	12.8	16
75	Systems-level effects of allosteric perturbations to a model molecular switch. Nature, 2021, 599, 152-157.	27.8	13
76	A Model for the Molecular Mechanism of an Engineered Light-Driven Protein Machine. Structure, 2016, 24, 576-584.	3.3	7
77	In support of the BMRB. Nature Structural and Molecular Biology, 2012, 19, 854-860.	8.2	6
78	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.	7.1	6
79	Design of Light-Controlled Protein Conformations and Functions. Methods in Molecular Biology, 2016, 1414, 197-211.	0.9	5
80	Advances in the Computational Design of Small-Molecule-Controlled Protein-Based Circuits for Synthetic Biology. Proceedings of the IEEE, 2022, 110, 659-674.	21.3	5
81	De novo protein fold families expand the designable ligand binding site space. PLoS Computational Biology, 2021, 17, e1009620.	3.2	3
82	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, .	7.1	2
83	Editorial overview: Engineering and design: Raising the bar through innovation and integration. Current Opinion in Structural Biology, 2014, 27, vi-viii.	5.7	0
84	Design of Multi-Specificity in Protein Interfaces. PLoS Computational Biology, 2005, preprint, e164.	3.2	0