List of Publications by Year in descending order

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TANIA KORTEMME

#	Article	IF	CITATIONS
1	Design principles of protein switches. Current Opinion in Structural Biology, 2022, 72, 71-78.	5.7	20
2	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
3	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
4	Recent advances in de novo protein design: Principles, methods, and applications. Journal of Biological Chemistry, 2021, 296, 100558.	3.4	120
5	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
6	Systems-level effects of allosteric perturbations to a model molecular switch. Nature, 2021, 599, 152-157.	27.8	13
7	De novo protein fold families expand the designable ligand binding site space. PLoS Computational Biology, 2021, 17, e1009620.	3.2	3
8	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Nature Communications, 2021, 12, 6947.	12.8	16
9	Comparison of Rosetta flexibleâ€backbone computational protein design methods on binding interactions. Proteins: Structure, Function and Bioinformatics, 2020, 88, 206-226.	2.6	27
10	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
11	New computational protein design methods for de novo small molecule binding sites. PLoS Computational Biology, 2020, 16, e1008178.	3.2	20
12	Comparative host-coronavirus protein interaction networks reveal pan-viral disease mechanisms. Science, 2020, 370, .	12.6	508
13	Expanding the space of protein geometries by computational design of de novo fold families. Science, 2020, 369, 1132-1136.	12.6	57
14	Better together: Elements of successful scientific software development in a distributed collaborative community. PLoS Computational Biology, 2020, 16, e1007507.	3.2	27
15	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	19.0	513
16	The Global Phosphorylation Landscape of SARS-CoV-2 Infection. Cell, 2020, 182, 685-712.e19.	28.9	825
17	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. Nature, 2020, 583, 459-468.	27.8	3,542
18	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

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19	Computational design of structured loops for new protein functions. Biological Chemistry, 2019, 400, 275-288.	2.5	25
20	Controlling CRISPR-Cas9 with ligand-activated and ligand-deactivated sgRNAs. Nature Communications, 2019, 10, 2127.	12.8	133
21	Computational design of a modular protein sense-response system. Science, 2019, 366, 1024-1028.	12.6	91
22	Quantitative mapping of protein-peptide affinity landscapes using spectrally encoded beads. ELife, 2019, 8, .	6.0	53
23	Flex ddG: Rosetta Ensemble-Based Estimation of Changes in Protein–Protein Binding Affinity upon Mutation. Journal of Physical Chemistry B, 2018, 122, 5389-5399.	2.6	192
24	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
25	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
26	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
27	Deconstruction of the Ras switching cycle through saturation mutagenesis. ELife, 2017, 6, .	6.0	95
28	Design of Light-Controlled Protein Conformations and Functions. Methods in Molecular Biology, 2016, 1414, 197-211.	0.9	5
29	A Model for the Molecular Mechanism of an Engineered Light-Driven Protein Machine. Structure, 2016, 24, 576-584.	3.3	7
30	Determination of ubiquitin fitness landscapes under different chemical stresses in a classroom setting. ELife, 2016, 5, .	6.0	71
31	A Web Resource for Standardized Benchmark Datasets, Metrics, and Rosetta Protocols for Macromolecular Modeling and Design. PLoS ONE, 2015, 10, e0130433.	2.5	85
32	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
33	Coupling Protein Side-Chain and Backbone Flexibility Improves the Re-design of Protein-Ligand Specificity. PLoS Computational Biology, 2015, 11, e1004335.	3.2	71
34	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
35	Editorial overview: Engineering and design: Raising the bar through innovation and integration. Current Opinion in Structural Biology, 2014, 27, vi-viii.	5.7	0
36	Design of a Phosphorylatable PDZ Domain with Peptide-Specific Affinity Changes. Structure, 2013, 21, 54-64.	3.3	17

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37	Design of a Photoswitchable Cadherin. Journal of the American Chemical Society, 2013, 135, 12516-12519.	13.7	22
38	Reprogramming an ATP-driven protein machine into a light-gated nanocage. Nature Nanotechnology, 2013, 8, 928-932.	31.5	55
39	Scientific Benchmarks for Guiding Macromolecular Energy Function Improvement. Methods in Enzymology, 2013, 523, 109-143.	1.0	195
40	Flexible Backbone Sampling Methods to Model and Design Protein Alternative Conformations. Methods in Enzymology, 2013, 523, 61-85.	1.0	44
41	Computational Protein Design Quantifies Structural Constraints on Amino Acid Covariation. PLoS Computational Biology, 2013, 9, e1003313.	3.2	35
42	Serverification of Molecular Modeling Applications: The Rosetta Online Server That Includes Everyone (ROSIE). PLoS ONE, 2013, 8, e63906.	2.5	348
43	Improvements to Robotics-Inspired Conformational Sampling in Rosetta. PLoS ONE, 2013, 8, e63090.	2.5	176
44	Amino-acid site variability among natural and designed proteins. PeerJ, 2013, 1, e211.	2.0	18
45	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
46	In support of the BMRB. Nature Structural and Molecular Biology, 2012, 19, 854-860.	8.2	6
47	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
48	Global landscape of HIV–human protein complexes. Nature, 2012, 481, 365-370.	27.8	651
49	Cost-Benefit Tradeoffs in Engineered <i>lac</i> Operons. Science, 2012, 336, 911-915.	12.6	90
50	Rosetta3. Methods in Enzymology, 2011, 487, 545-574.	1.0	1,620
51	Assessment of flexible backbone protein design methods for sequence library prediction in the the the therapeutic antibody Herceptin–HER2 interface. Protein Science, 2011, 20, 1082-1089.	7.6	30
52	Predicting the Tolerated Sequences for Proteins and Protein Interfaces Using RosettaBackrub Flexible Backbone Design. PLoS ONE, 2011, 6, e20451.	2.5	94
53	Designing ensembles in conformational and sequence space to characterize and engineer proteins. Current Opinion in Structural Biology, 2010, 20, 377-384.	5.7	26
54	SNX27 mediates PDZ-directed sorting from endosomes to the plasma membrane. Journal of Cell Biology, 2010, 190, 565-574.	5.2	222

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55	RosettaBackrub–a web server for flexible backbone protein structure modeling and design. Nucleic Acids Research, 2010, 38, W569-W575.	14.5	110
56	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
57	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
58	Backbone flexibility in computational protein design. Current Opinion in Biotechnology, 2009, 20, 420-428.	6.6	93
59	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
60	Computer-aided design of functional protein interactions. Nature Chemical Biology, 2009, 5, 797-807.	8.0	144
61	Sub-angstrom accuracy in protein loop reconstruction by robotics-inspired conformational sampling. Nature Methods, 2009, 6, 551-552.	19.0	408
62	Prediction of Protein-Protein Interface Sequence Diversity Using Flexible Backbone Computational Protein Design. Structure, 2008, 16, 1777-1788.	3.3	73
63	A New Twist in TCR Diversity Revealed by a Forbidden αβ TCR. Journal of Molecular Biology, 2008, 375, 1306-1319.	4.2	21
64	A Simple Model of Backbone Flexibility Improves Modeling of Side-chain Conformational Variability. Journal of Molecular Biology, 2008, 380, 757-774.	4.2	67
65	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
66	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
67	Design of Multi-Specificity in Protein Interfaces. PLoS Computational Biology, 2007, 3, e164.	3.2	95
68	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
69	Ca2+ Indicators Based on Computationally Redesigned Calmodulin-Peptide Pairs. Chemistry and Biology, 2006, 13, 521-530.	6.0	455
70	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
71	Potential Functions for Hydrogen Bonds in Protein Structure Prediction and Design. Advances in Protein Chemistry, 2005, 72, 1-38.	4.4	57
72	Design of Multi-Specificity in Protein Interfaces. PLoS Computational Biology, 2005, preprint, e164.	3.2	0

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73	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
74	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
75	Computational redesign of protein-protein interaction specificity. Nature Structural and Molecular Biology, 2004, 11, 371-379.	8.2	279
76	Computational design of protein–protein interactions. Current Opinion in Chemical Biology, 2004, 8, 91-97.	6.1	213
77	Computational Alanine Scanning of Protein-Protein Interfaces. Science Signaling, 2004, 2004, pl2-pl2.	3.6	471
78	Symmetry Recognizing Asymmetry. Structure, 2003, 11, 411-422.	3.3	99
79	Evaluation of Models of Electrostatic Interactions in Proteins. Journal of Physical Chemistry B, 2003, 107, 2075-2090.	2.6	50
80	An Orientation-dependent Hydrogen Bonding Potential Improves Prediction of Specificity and Structure for Proteins and Protein–Protein Complexes. Journal of Molecular Biology, 2003, 326, 1239-1259.	4.2	460
81	Convergent Mechanisms for Recognition of Divergent Cytokines by the Shared Signaling Receptor gp130. Molecular Cell, 2003, 12, 577-589.	9.7	131
82	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
83	Design, Activity, and Structure of a Highly Specific Artificial Endonuclease. Molecular Cell, 2002, 10, 895-905.	9.7	218
84	The design of linear peptides that fold as monomeric Î ² -sheet structures. Current Opinion in Structural Biology, 1999, 9, 487-493.	5.7	128