David Baker

List of Publications by Year in Descending Order

657 papers	75,982 citations	151 h-index	254 g-index
714 ext. papers	90,218 ext. citations	14.1 avg, IF	8.14 L-index

#	Paper	IF	Citations
657	Deep learning and protein structure modeling.. *Nature Methods*, **2022**, 19, 13-14	21.6	8
656	Reconfigurable asymmetric protein assemblies through implicit negative design.. *Science*, **2022**, 375, eabj7662	33.3	4
655	Interpreting neural networks for biological sequences by learning stochastic masks. *Nature Machine Intelligence*, **2022**, 4, 41-54	22.5	0
654	Interpreting Potts and Transformer Protein Models Through the Lens of Simplified Attention. *Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing*, **2022**, 27, 34-45	1.3	
653	Natural and Designed Proteins Inspired by Extremotolerant Organisms Can Form Condensates and Attenuate Apoptosis in Human Cells.. *ACS Synthetic Biology*, **2022**,	5.7	1
652	Competitive Displacement of De Novo Designed HeteroDimers Can Reversibly Control ProteinProtein Interactions and Implement Feedback in Synthetic Circuits **2022**, 1, 91-100		1
651	De novo design and directed folding of disulfide-bridged peptide heterodimers.. *Nature Communications*, **2022**, 13, 1539	17.4	0
650	Large-scale design and refinement of stable proteins using sequence-only models.. *PLoS ONE*, **2022**, 17, e0265020	3.7	0
649	Design of protein binding proteins from target structure alone.. *Nature*, **2022**,	50.4	13
648	Multivalent designed proteins neutralize SARS-CoV-2 variants of concern and confer protection against infection in mice.. *Science Translational Medicine*, **2022**, 14, eabn1252	17.5	3
647	Rotational dynamics and transition mechanisms of surface-adsorbed proteins.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2020242119	11.5	1
646	Computational design of mechanically coupled axle-rotor protein assemblies.. *Science*, **2022**, 376, 383-390	33.3	2
645	The road to fully programmable protein catalysis. *Nature*, **2022**, 606, 49-58	50.4	13
644	Computed structures of core eukaryotic protein complexes. *Science*, **2021**, 374, eabm4805	33.3	51
643	The trRosetta server for fast and accurate protein structure prediction. *Nature Protocols*, **2021**, 16, 5634-5651	13.1	36
642	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. *Nature Communications*, **2021**, 12, 6947	17.4	0
641	De novo protein design by deep network hallucination. *Nature*, **2021**,	50.4	33

640	F-domain valency determines outcome of signaling through the angiopoietin pathway. *EMBO Reports*, **2021**, 22, e53471	6.5	4
639	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
638	Ultrapotent miniproteins targeting the receptor-binding domain protect against SARS-CoV-2 infection and disease in mice **2021**,		1
637	Isolating Conformers to Assess Dynamics of Peptidic Catalysts Using Computationally Designed Macrocyclic Peptides. *ACS Catalysis*, **2021**, 11, 4395-4400	13.1	4
636	Protein sequence design by conformational landscape optimization. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	29
635	O-GlcNAc modification of small heat shock proteins enhances their anti-amyloid chaperone activity. *Nature Chemistry*, **2021**, 13, 441-450	17.6	18
634	Quadrivalent influenza nanoparticle vaccines induce broad protection. *Nature*, **2021**, 592, 623-628	50.4	40
633	Sentinel cells enable genetic detection of SARS-CoV-2 Spike protein **2021**,		1
632	Transferrin receptor targeting by de novo sheet extension. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	6
631	Disentangling Rotational Dynamics and Ordering Transitions in a System of Self-Organizing Protein Nanorods Rotationally Invariant Latent Representations. *ACS Nano*, **2021**, 15, 6471-6480	16.7	7
630	Designed proteins assemble antibodies into modular nanocages. *Science*, **2021**, 372,	33.3	35
629	Design of multi-scale protein complexes by hierarchical building block fusion. *Nature Communications*, **2021**, 12, 2294	17.4	14
628	COVID-19 Rehabilitation With Herbal Medicine and Cardiorespiratory Exercise: Protocol for a Clinical Study. *JMIR Research Protocols*, **2021**, 10, e25556	2	2
627	Ion-dependent protein-surface interactions from intrinsic solvent response. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	5
626	Detection of antibodies neutralizing historical and emerging SARS-CoV-2 strains using a thermodynamically coupled de novo biosensor system **2021**,		1
625	Role of backbone strain in de novo design of complex α/β protein structures. *Nature Communications*, **2021**, 12, 3921	17.4	9
624	Anchor extension: a structure-guided approach to design cyclic peptides targeting enzyme active sites. *Nature Communications*, **2021**, 12, 3384	17.4	12
623	Generation of ordered protein assemblies using rigid three-body fusion. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	6

622	Engineering Biomolecular Self-Assembly at Solid-Liquid Interfaces. *Advanced Materials*, **2021**, 33, e1905784	24	11
621	Perturbing the energy landscape for improved packing during computational protein design. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 436-449	4.2	22
620	Quantifying the Dynamics of Protein Self-Organization Using Deep Learning Analysis of Atomic Force Microscopy Data. *Nano Letters*, **2021**, 21, 158-165	11.5	7
619	Alignment of Au nanorods along designed protein nanofibers studied with automated image analysis. *Soft Matter*, **2021**, 17, 6109-6115	3.6	3
618	Design of biologically active binary protein 2D materials. *Nature*, **2021**, 589, 468-473	50.4	33
617	De novo design of modular and tunable protein biosensors. *Nature*, **2021**, 591, 482-487	50.4	53
616	Incorporation of sensing modalities into de novo designed fluorescence-activating proteins. *Nature Communications*, **2021**, 12, 856	17.4	7
615	Improved protein structure refinement guided by deep learning based accuracy estimation. *Nature Communications*, **2021**, 12, 1340	17.4	50
614	Force Field Optimization Guided by Small Molecule Crystal Lattice Data Enables Consistent Sub-Angstrom Protein-Ligand Docking. *Journal of Chemical Theory and Computation*, **2021**, 17, 2000-2010	6.4	12
613	De novo design of transmembrane barrels. *Science*, **2021**, 371,	33.3	25
612	Protein sequence optimization with a pairwise decomposable penalty for buried unsatisfied hydrogen bonds. *PLoS Computational Biology*, **2021**, 17, e1008061	5	8
611	Computational design of a synthetic PD-1 agonist. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	9
610	Importance of Substrate-Particle Repulsion for Protein-Templated Assembly of Metal Nanoparticles. *Langmuir*, **2021**, 37, 9111-9119	4	1
609	Accurate prediction of protein structures and interactions using a three-track neural network. *Science*, **2021**, 373, 871-876	33.3	522
608	Multivalent designed proteins protect against SARS-CoV-2 variants of concern **2021**,		4
607	Ultrapotent miniproteins targeting the SARS-CoV-2 receptor-binding domain protect against infection and disease. *Cell Host and Microbe*, **2021**, 29, 1151-1161.e5	23.4	11
606	Protein tertiary structure prediction and refinement using deep learning and Rosetta in CASP14. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 1722-1733	4.2	9
605	Protein oligomer modeling guided by predicted interchain contacts in CASP14. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 1824-1833	4.2	4

604	Polyclonal antibody responses to HIV Env immunogens resolved using cryoEM. *Nature Communications*, **2021**, 12, 4817	17.4	8
603	The Stability Landscape of de novo TIM Barrels Explored by a Modular Design Approach. *Journal of Molecular Biology*, **2021**, 433, 167153	6.5	3
602	De novo design of tyrosine and serine kinase-driven protein switches. *Nature Structural and Molecular Biology*, **2021**, 28, 762-770	17.6	5
601	Super-enhancer-based identification of a BATF3/IL-2R-module reveals vulnerabilities in anaplastic large cell lymphoma. *Nature Communications*, **2021**, 12, 5577	17.4	1
600	Stapled Hairpins Featuring 4-Mercaptoproline. *Journal of the American Chemical Society*, **2021**, 143, 15039-15044	16.4	0
599	Treatment of experimental anthrax with pegylated circularly permuted capsule depolymerase. *Science Translational Medicine*, **2021**, 13, eabh1682	17.5	0
598	Engineering an efficient and enantioselective enzyme for the Morita-Baylis-Hillman reaction.. *Nature Chemistry*, **2021**,	17.6	7
597	Better together: Elements of successful scientific software development in a distributed collaborative community. *PLoS Computational Biology*, **2020**, 16, e1007507	5	15
596	Macromolecular modeling and design in Rosetta: recent methods and frameworks. *Nature Methods*, **2020**, 17, 665-680	21.6	165
595	De novo design of protein logic gates. *Science*, **2020**, 368, 78-84	33.3	88
594	Sequence-Structure-Binding Relationships Reveal Adhesion Behavior of the Car9 Solid-Binding Peptide: An Integrated Experimental and Simulation Study. *Journal of the American Chemical Society*, **2020**, 142, 2355-2363	16.4	11
593	Rapid online buffer exchange for screening of proteins, protein complexes and cell lysates by native mass spectrometry. *Nature Protocols*, **2020**, 15, 1132-1157	18.8	46
592	Modular repeat protein sculpting using rigid helical junctions. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 8870-8875	11.5	21
591	Computational design of closely related proteins that adopt two well-defined but structurally divergent folds. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 7208-7215	11.5	27
590	Deep learning enables the atomic structure determination of the Fanconi Anemia core complex from cryoEM. *IUCrJ*, **2020**, 7, 881-892	4.7	5
589	Tailored design of protein nanoparticle scaffolds for multivalent presentation of viral glycoprotein antigens. *ELife*, **2020**, 9,	8.9	51
588	design of modular and tunable allosteric biosensors **2020**,		6
587	De novo design of picomolar SARS-CoV-2 miniprotein inhibitors **2020**,		9

586	F-domain valency determines outcome of signaling through the angiopoietin pathway **2020**,		28
585	Designed proteins assemble antibodies into modular nanocages **2020**,		5
584	Parallelized identification of on- and off-target protein interactions.. *Molecular Systems Design and Engineering*, **2020**, 5, 349-357	4.6	0
583	Improved protein structure prediction using predicted interresidue orientations. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 1496-1503	11.5	496
582	Design and structure of two new protein cages illustrate successes and ongoing challenges in protein engineering. *Protein Science*, **2020**, 29, 919-929	6.3	9
581	Computational design of mixed chirality peptide macrocycles with internal symmetry. *Protein Science*, **2020**, 29, 2433-2445	6.3	9
580	A Potent Anti-Malarial Human Monoclonal Antibody Targets Circumsporozoite Protein Minor Repeats and Neutralizes Sporozoites in the Liver. *Immunity*, **2020**, 53, 733-744.e8	32.3	29
579	Next-Generation Surrogate Wnts Support Organoid Growth and Deconvolute Frizzled Pleiotropy In Vivo. *Cell Stem Cell*, **2020**, 27, 840-851.e6	18	33
578	Tight and specific lanthanide binding in a de novo TIM barrel with a large internal cavity designed by symmetric domain fusion. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 30362-30369	11.5	17
577	Structural and functional evaluation of de novo-designed, two-component nanoparticle carriers for HIV Env trimer immunogens. *PLoS Pathogens*, **2020**, 16, e1008665	7.6	25
576	Computational design of transmembrane pores. *Nature*, **2020**, 585, 129-134	50.4	56
575	De novo design of picomolar SARS-CoV-2 miniprotein inhibitors. *Science*, **2020**, 370, 426-431	33.3	219
574	Conditional Recruitment to a DNA-Bound CRISPR-Cas Complex Using a Colocalization-Dependent Protein Switch. *ACS Synthetic Biology*, **2020**, 9, 2316-2323	5.7	1
573	Designed protein logic to target cells with precise combinations of surface antigens. *Science*, **2020**, 369, 1637-1643	33.3	48
572	Targeting HIV Env immunogens to B cell follicles in nonhuman primates through immune complex or protein nanoparticle formulations. *Npj Vaccines*, **2020**, 5, 72	9.5	20
571	An enumerative algorithm for de novo design of proteins with diverse pocket structures. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 22135-22145	11.5	28
570	Self-assembly-based posttranslational protein oscillators. *Science Advances*, **2020**, 6,	14.3	1
569	Protein contact prediction using metagenome sequence data and residual neural networks. *Bioinformatics*, **2020**, 36, 41-48	7.2	43

568	Structural and functional evaluation of de novo-designed, two-component nanoparticle carriers for HIV Env trimer immunogens **2020**, 16, e1008665		
567	Structural and functional evaluation of de novo-designed, two-component nanoparticle carriers for HIV Env trimer immunogens **2020**, 16, e1008665		
566	Structural and functional evaluation of de novo-designed, two-component nanoparticle carriers for HIV Env trimer immunogens **2020**, 16, e1008665		
565	Structural and functional evaluation of de novo-designed, two-component nanoparticle carriers for HIV Env trimer immunogens **2020**, 16, e1008665		
564	Improving the Efficiency of Ligand-Binding Protein Design with Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2019**, 15, 5703-5715	6.4	10
563	Multi-input chemical control of protein dimerization for programming graded cellular responses. *Nature Biotechnology*, **2019**, 37, 1209-1216	44.5	21
562	Enhancing and shaping the immunogenicity of native-like HIV-1 envelope trimers with a two-component protein nanoparticle. *Nature Communications*, **2019**, 10, 4272	17.4	80
561	Functional expression and characterization of the envelope glycoprotein E1E2 heterodimer of hepatitis C virus. *PLoS Pathogens*, **2019**, 15, e1007759	7.6	15
560	Intratumoral activation of the necroptotic pathway components RIPK1 and RIPK3 potentiates antitumor immunity. *Science Immunology*, **2019**, 4,	28	114
559	De novo protein design by citizen scientists. *Nature*, **2019**, 570, 390-394	50.4	63
558	Topological control of cytokine receptor signaling induces differential effects in hematopoiesis. *Science*, **2019**, 364,	33.3	47
557	Multimerization of an Alcohol Dehydrogenase by Fusion to a Designed Self-Assembling Protein Results in Enhanced Bioelectrocatalytic Operational Stability. *ACS Applied Materials & Interfaces*, **2019**, 11, 20022-20028	9.5	5
556	Receptor subtype discrimination using extensive shape complementary designed interfaces. *Nature Structural and Molecular Biology*, **2019**, 26, 407-414	17.6	19
555	De novo design of tunable, pH-driven conformational changes. *Science*, **2019**, 364, 658-664	33.3	60
554	Self-Assembling 2D Arrays with de Novo Protein Building Blocks. *Journal of the American Chemical Society*, **2019**, 141, 8891-8895	16.4	24
553	Networks of electrostatic and hydrophobic interactions modulate the complex folding free energy surface of a designed protein. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 6806-6811	11.5	16
552	Induction of Potent Neutralizing Antibody Responses by a Designed Protein Nanoparticle Vaccine for Respiratory Syncytial Virus. *Cell*, **2019**, 176, 1420-1431.e17	56.2	190
551	An integrated device for the rapid and sensitive detection of the influenza hemagglutinin. *Lab on A Chip*, **2019**, 19, 885-896	7.2	14

550	A cell-free platform for the prenylation of natural products and application to cannabinoid production. *Nature Communications*, **2019**, 10, 565	17.4	49
549	High-accuracy refinement using Rosetta in CASP13. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 1276-1282	4.2	26
548	Controlling protein assembly on inorganic crystals through designed protein interfaces. *Nature*, **2019**, 571, 251-256	50.4	55
547	Modular and tunable biological feedback control using a de novo protein switch. *Nature*, **2019**, 572, 265-269	50.4	58
546	De novo design of bioactive protein switches. *Nature*, **2019**, 572, 205-210	50.4	113
545	Computationally designed protein activation. *National Science Review*, **2019**, 6, 609-610	10.8	
544	Template-based modeling by ClusPro in CASP13 and the potential for using co-evolutionary information in docking. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 1241-1248	4.2	7
543	A computational method for design of connected catalytic networks in proteins. *Protein Science*, **2019**, 28, 2036-2041	6.3	19
542	Protein interaction networks revealed by proteome coevolution. *Science*, **2019**, 365, 185-189	33.3	112
541	De novo design of a homo-trimeric amantadine-binding protein. *ELife*, **2019**, 8,	8.9	10
540	What has de novo protein design taught us about protein folding and biophysics?. *Protein Science*, **2019**, 28, 678-683	6.3	81
539	De Novo Carborane-Containing Macrocyclic Peptides Targeting Human Epidermal Growth Factor Receptor. *Journal of the American Chemical Society*, **2019**, 141, 19193-19197	16.4	24
538	Building de novo cryo-electron microscopy structures collaboratively with citizen scientists. *PLoS Biology*, **2019**, 17, e3000472	9.7	9
537	Programmable design of orthogonal protein heterodimers. *Nature*, **2019**, 565, 106-111	50.4	87
536	De novo design of potent and selective mimics of IL-2 and IL-15. *Nature*, **2019**, 565, 186-191	50.4	184
535	Structurally Mapping Endogenous Heme in the CcmCDE Membrane Complex for Cytochrome c Biogenesis. *Journal of Molecular Biology*, **2018**, 430, 1065-1080	6.5	11
534	Accurate computational design of multipass transmembrane proteins. *Science*, **2018**, 359, 1042-1046	33.3	93
533	Selective targeting of engineered T cells using orthogonal IL-2 cytokine-receptor complexes. *Science*, **2018**, 359, 1037-1042	33.3	149

532	Protein homology model refinement by large-scale energy optimization. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 3054-3059	11.5	49
531	Rapid Sampling of Hydrogen Bond Networks for Computational Protein Design. *Journal of Chemical Theory and Computation*, **2018**, 14, 2751-2760	6.4	24
530	Structures and disulfide cross-linking of de novo designed therapeutic mini-proteins. *FEBS Journal*, **2018**, 285, 1783-1785	5.7	6
529	Confirmation of intersubunit connectivity and topology of designed protein complexes by native MS. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 1268-1273	11.5	40
528	Improved Free-Energy Landscape Quantification Illustrated with a Computationally Designed Protein-Ligand Interaction. *ChemPhysChem*, **2018**, 19, 19-23	3.2	4
527	Protein structure prediction using Rosetta in CASP12. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86 Suppl 1, 113-121	4.2	63
526	Elfin: An algorithm for the computational design of custom three-dimensional structures from modular repeat protein building blocks. *Journal of Structural Biology*, **2018**, 201, 100-107	3.4	6
525	Automatic structure prediction of oligomeric assemblies using Robetta in CASP12. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86 Suppl 1, 283-291	4.2	29
524	Extreme stability in de novo-designed repeat arrays is determined by unusually stable short-range interactions. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 7539-7544	11.5	18
523	An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. *Scientific Reports*, **2018**, 8, 9939	4.9	16
522	Discovery and engineering of enhanced SUMO protease enzymes. *Journal of Biological Chemistry*, **2018**, 293, 13224-13233	5.4	12
521	Cytosolic expression, solution structures, and molecular dynamics simulation of genetically encodable disulfide-rich de novo designed peptides. *Protein Science*, **2018**, 27, 1611-1623	6.3	11
520	De novo design of self-assembling helical protein filaments. *Science*, **2018**, 362, 705-709	33.3	78
519	Unintended specificity of an engineered ligand-binding protein facilitated by unpredicted plasticity of the protein fold. *Protein Engineering, Design and Selection*, **2018**, 31, 375-387	1.9	5
518	Simple yet functional phosphate-loop proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E11943-E11950	11.5	44
517	De novo design of a non-local β-sheet protein with high stability and accuracy. *Nature Structural and Molecular Biology*, **2018**, 25, 1028-1034	17.6	54
516	Engineered Biosensors from Dimeric Ligand-Binding Domains. *ACS Synthetic Biology*, **2018**, 7, 2457-2467	5.7	15
515	De novo design of a fluorescence-activating β-barrel. *Nature*, **2018**, 561, 485-491	50.4	156

514	Protein structure determination using metagenome sequence data. *Science*, **2017**, 355, 294-298	33.3	346
513	Principles for designing proteins with cavities formed by curved β sheets. *Science*, **2017**, 355, 201-206	33.3	82
512	Overcoming an optimization plateau in the directed evolution of highly efficient nerve agent bioscavengers. *Protein Engineering, Design and Selection*, **2017**, 30, 333-345	1.9	41
511	The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design. *Journal of Chemical Theory and Computation*, **2017**, 13, 3031-3048	6.4	486
510	Rapid Diagnostic Assay for Intact Influenza Virus Using a High Affinity Hemagglutinin Binding Protein. *Analytical Chemistry*, **2017**, 89, 6608-6615	7.8	12
509	Foldit Standalone: a video game-derived protein structure manipulation interface using Rosetta. *Bioinformatics*, **2017**, 33, 2765-2767	7.2	44
508	Surrogate Wnt agonists that phenocopy canonical Wnt and β-catenin signalling. *Nature*, **2017**, 545, 234-237	50.4	165
507	Computational design of trimeric influenza-neutralizing proteins targeting the hemagglutinin receptor binding site. *Nature Biotechnology*, **2017**, 35, 667-671	44.5	84
506	Computational design of self-assembling cyclic protein homo-oligomers. *Nature Chemistry*, **2017**, 9, 353-360	17.6	78
505	High-throughput characterization of protein-protein interactions by reprogramming yeast mating. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 12166-12171	11.5	27
504	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
503	Massively parallel de novo protein design for targeted therapeutics. *Nature*, **2017**, 550, 74-79	50.4	235
502	First critical repressive H3K27me3 marks in embryonic stem cells identified using designed protein inhibitor. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 10125-10130	11.5	24
501	Origins of coevolution between residues distant in protein 3D structures. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 9122-9127	11.5	92
500	Global analysis of protein folding using massively parallel design, synthesis, and testing. *Science*, **2017**, 357, 168-175	33.3	241
499	Cyclic oligomer design with de novo β-proteins. *Protein Science*, **2017**, 26, 2187-2194	6.3	7
498	Evolution of a designed protein assembly encapsulating its own RNA genome. *Nature*, **2017**, 552, 415-420	50.4	116
497	Direction of actin flow dictates integrin LFA-1 orientation during leukocyte migration. *Nature Communications*, **2017**, 8, 2047	17.4	55

496	Comprehensive computational design of ordered peptide macrocycles. *Science*, **2017**, 358, 1461-1466	33.3	96
495	Cryo-EM structure of the protein-conducting ERAD channel Hrd1 in complex with Hrd3. *Nature*, **2017**, 548, 352-355	50.4	117
494	Emergence of a catalytic tetrad during evolution of a highly active artificial aldolase. *Nature Chemistry*, **2017**, 9, 50-56	17.6	184
493	A computationally engineered RAS rheostat reveals RAS-ERK signaling dynamics. *Nature Chemical Biology*, **2017**, 13, 119-126	11.7	15
492	Mammalian display screening of diverse cystine-dense peptides for difficult to drug targets. *Nature Communications*, **2017**, 8, 2244	17.4	34
491	Applications of contact predictions to structural biology. *IUCrJ*, **2017**, 4, 291-300	4.7	30
490	Computational design of environmental sensors for the potent opioid fentanyl. *ELife*, **2017**, 6,	8.9	44
489	Sampling and energy evaluation challenges in ligand binding protein design. *Protein Science*, **2017**, 26, 2426-2437	6.3	23
488	Immobilizing affinity proteins to nitrocellulose: a toolbox for paper-based assay developers. *Analytical and Bioanalytical Chemistry*, **2016**, 408, 1335-46	4.4	58
487	CSAR Benchmark Exercise 2013: Evaluation of Results from a Combined Computational Protein Design, Docking, and Scoring/Ranking Challenge. *Journal of Chemical Information and Modeling*, **2016**, 56, 1022-31	6.1	36
486	Accurate de novo design of hyperstable constrained peptides. *Nature*, **2016**, 538, 329-335	50.4	231
485	The coming of age of de novo protein design. *Nature*, **2016**, 537, 320-7	50.4	697
484	Accurate design of megadalton-scale two-component icosahedral protein complexes. *Science*, **2016** , 353, 389-94	33.3	322
483	Multivalent Display of Antifreeze Proteins by Fusion to Self-Assembling Protein Cages Enhances Ice-Binding Activities. *Biochemistry*, **2016**, 55, 6811-6820	3.2	23
482	Determining crystal structures through crowdsourcing and coursework. *Nature Communications*, **2016**, 7, 12549	17.4	35
481	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
480	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. *Journal of Cheminformatics*, **2016**, 8, 18	8.6	
479	Design of a hyperstable 60-subunit protein dodecahedron. [corrected]. *Nature*, **2016**, 535, 136-9	50.4	243

478	Multiplex pairwise assembly of array-derived DNA oligonucleotides. *Nucleic Acids Research*, **2016**, 44, e43	20.1	31
477	Engineering an allosteric transcription factor to respond to new ligands. *Nature Methods*, **2016**, 13, 177-83	21.6	184
476	De novo design of a four-fold symmetric TIM-barrel protein with atomic-level accuracy. *Nature Chemical Biology*, **2016**, 12, 29-34	11.7	151
475	Catalytic efficiencies of directly evolved phosphotriesterase variants with structurally different organophosphorus compounds in vitro. *Archives of Toxicology*, **2016**, 90, 2711-2724	5.8	35
474	Protection of the Furin Cleavage Site in Low-Toxicity Immunotoxins Based on Pseudomonas Exotoxin A. *Toxins*, **2016**, 8,	4.9	17
473	Computationally designed high specificity inhibitors delineate the roles of BCL2 family proteins in cancer. *ELife*, **2016**, 5,	8.9	52
472	A Computationally Designed Hemagglutinin Stem-Binding Protein Provides In Vivo Protection from Influenza Independent of a Host Immune Response. *PLoS Pathogens*, **2016**, 12, e1005409	7.6	36
471	Structure prediction using sparse simulated NOE restraints with Rosetta in CASP11. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84 Suppl 1, 181-8	4.2	11
470	CASP11 refinement experiments with ROSETTA. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84 Suppl 1, 314-22	4.2	18
469	Introduction of a polar core into the de novo designed protein Top7. *Protein Science*, **2016**, 25, 1299-307	6.3	4
468	Designed protein aggregates entrapping carbon nanotubes for bioelectrochemical oxygen reduction. *Biotechnology and Bioengineering*, **2016**, 113, 2321-7	4.9	8
467	Improved de novo structure prediction in CASP11 by incorporating coevolution information into Rosetta. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84 Suppl 1, 67-75	4.2	82
466	Computational design of a homotrimeric metalloprotein with a trisbipyridyl core. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 15012-15017	11.5	33
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