David Baker

List of Publications by Citations

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	Contact order, transition state placement and the refolding rates of single domain proteins. *Journal of Molecular Biology*, **1998**, 277, 985-94	6.5	1303
656	Protein structure prediction and analysis using the Robetta server. *Nucleic Acids Research*, **2004**, 32, W526-31	6.3	1239
655	Design of a novel globular protein fold with atomic-level accuracy. *Science*, **2003**, 302, 1364-8	33.3	1237
654	Protein structure prediction and structural genomics. *Science*, **2001**, 294, 93-6	33.3	1235
653	ROSETTA3: an object-oriented software suite for the simulation and design of macromolecules. *Methods in Enzymology*, **2011**, 487, 545-74	1.7	1216
652	Protein structure prediction using Rosetta. *Methods in Enzymology*, **2004**, 383, 66-93	1.7	1142
651	Assembly of protein tertiary structures from fragments with similar local sequences using simulated annealing and Bayesian scoring functions. *Journal of Molecular Biology*, **1997**, 268, 209-25	6.5	1108
650	Quantitative reactivity profiling predicts functional cysteines in proteomes. *Nature*, **2010**, 468, 790-5	50.4	1056
649	Kemp elimination catalysts by computational enzyme design. *Nature*, **2008**, 453, 190-5	50.4	977
648	De novo computational design of retro-aldol enzymes. *Science*, **2008**, 319, 1387-91	33.3	892
647	Protein-protein docking with simultaneous optimization of rigid-body displacement and side-chain conformations. *Journal of Molecular Biology*, **2003**, 331, 281-99	6.5	858
646	Improving physical realism, stereochemistry, and side-chain accuracy in homology modeling: Four approaches that performed well in CASP8. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77 Suppl 9, 114-22	4.2	844
645	Predicting protein structures with a multiplayer online game. *Nature*, **2010**, 466, 756-60	50.4	821
644	The coming of age of de novo protein design. *Nature*, **2016**, 537, 320-7	50.4	697
643	Macromolecular modeling with rosetta. *Annual Review of Biochemistry*, **2008**, 77, 363-82	29.1	693
642	Toward high-resolution de novo structure prediction for small proteins. *Science*, **2005**, 309, 1868-71	33.3	686
641	Native protein sequences are close to optimal for their structures. *Proceedings of the National Academy of Sciences of the United States of America*, **2000**, 97, 10383-8	11.5	671

640	Consistent blind protein structure generation from NMR chemical shift data. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 4685-90	11.5	665
639	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
638	Computational design of an enzyme catalyst for a stereoselective bimolecular Diels-Alder reaction. *Science*, **2010**, 329, 309-13	33.3	652
637	High-resolution comparative modeling with RosettaCM. *Structure*, **2013**, 21, 1735-42	5.2	649
636	A surprising simplicity to protein folding. *Nature*, **2000**, 405, 39-42	50.4	648
635	An engineered microbial platform for direct biofuel production from brown macroalgae. *Science*, **2012**, 335, 308-13	33.3	534
634	Accurate prediction of protein structures and interactions using a three-track neural network. *Science*, **2021**, 373, 871-876	33.3	522
633	Rational HIV immunogen design to target specific germline B cell receptors. *Science*, **2013**, 340, 711-6	33.3	519
632	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
631	The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design. *Journal of Chemical Theory and Computation*, **2017**, 13, 3031-3048	6.4	486
630	Computational design of self-assembling protein nanomaterials with atomic level accuracy. *Science*, **2012**, 336, 1171-4	33.3	473
629	Computational design of proteins targeting the conserved stem region of influenza hemagglutinin. *Science*, **2011**, 332, 816-21	33.3	441
628	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
627	Assessing the utility of coevolution-based residue-residue contact predictions in a sequence- and structure-rich era. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 15674-9	11.5	423
626	High-resolution microtubule structures reveal the structural transitions in Ɓtubulin upon GTP hydrolysis. *Cell*, **2014**, 157, 1117-29	56.2	422
625	Accurate design of co-assembling multi-component protein nanomaterials. *Nature*, **2014**, 510, 103-8	50.4	403
624	Ca2+ indicators based on computationally redesigned calmodulin-peptide pairs. *Chemistry and Biology*, **2006**, 13, 521-30		402
623	Robust and accurate prediction of residue-residue interactions across protein interfaces using evolutionary information. *ELife*, **2014**, 3, e02030	8.9	397

622	Principles for designing ideal protein structures. *Nature*, **2012**, 491, 222-7	50.4	391
621	Role of conformational sampling in computing mutation-induced changes in protein structure and stability. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 830-8	4.2	379
620	Proof of principle for epitope-focused vaccine design. *Nature*, **2014**, 507, 201-6	50.4	365
619	Computational alanine scanning of protein-protein interfaces. *Science Signaling*, **2004**, 2004, pl2	8.8	361
618	Computational enzyme design. *Angewandte Chemie - International Edition*, **2013**, 52, 5700-25	16.4	351
617	High-resolution mapping of protein sequence-function relationships. *Nature Methods*, **2010**, 7, 741-6	21.6	350
616	Protein structure determination using metagenome sequence data. *Science*, **2017**, 355, 294-298	33.3	346
615	Structure prediction for CASP8 with all-atom refinement using Rosetta. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77 Suppl 9, 89-99	4.2	342
614	Structure-based design of non-natural amino-acid inhibitors of amyloid fibril formation. *Nature*, **2011**, 475, 96-100	50.4	341
613	Topology, stability, sequence, and length: defining the determinants of two-state protein folding kinetics. *Biochemistry*, **2000**, 39, 11177-83	3.2	340
612	Improved recognition of native-like protein structures using a combination of sequence-dependent and sequence-independent features of proteins. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 82-95	4.2	337
611	ROSETTALIGAND: protein-small molecule docking with full side-chain flexibility. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 538-48	4.2	336
610	Automated de novo prediction of native-like RNA tertiary structures. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 14664-9	11.5	334
609	Ab initio protein structure prediction of CASP III targets using ROSETTA. *Proteins: Structure, Function and Bioinformatics*, **1999**, 37, 171-176	4.2	334
608	Protein-protein docking with backbone flexibility. *Journal of Molecular Biology*, **2007**, 373, 503-19	6.5	329
607	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
606	Role of neurogenic genes in establishment of follicle cell fate and oocyte polarity during oogenesis in Drosophila. *Cell*, **1991**, 66, 433-49	56.2	325
605	Experiment and theory highlight role of native state topology in SH3 folding. *Nature Structural Biology*, **1999**, 6, 1016-24		323

604	Accurate design of megadalton-scale two-component icosahedral protein complexes. *Science*, **2016**, 353, 389-94	33.3	322
603	Critical role of beta-hairpin formation in protein G folding. *Nature Structural Biology*, **2000**, 7, 669-73		320
602	Crystal structure of a monomeric retroviral protease solved by protein folding game players. *Nature Structural and Molecular Biology*, **2011**, 18, 1175-7	17.6	316
601	Reconstitution of SEC gene product-dependent intercompartmental protein transport. *Cell*, **1988**, 54, 335-44	56.2	312
600	RosettaScripts: a scripting language interface to the Rosetta macromolecular modeling suite. *PLoS ONE*, **2011**, 6, e20161	3.7	311
599	RosettaLigand docking with full ligand and receptor flexibility. *Journal of Molecular Biology*, **2009**, 385, 381-92	6.5	309
598	Computational thermostabilization of an enzyme. *Science*, **2005**, 308, 857-60	33.3	303
597	Computational design of ligand-binding proteins with high affinity and selectivity. *Nature*, **2013**, 501, 212-216	50.4	299
596	Prediction of local structure in proteins using a library of sequence-structure motifs. *Journal of Molecular Biology*, **1998**, 281, 565-77	6.5	291
595	Algorithm discovery by protein folding game players. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 18949-53	11.5	289
594	Contact order revisited: influence of protein size on the folding rate. *Protein Science*, **2003**, 12, 2057-62	6.3	289
593	A protein-folding reaction under kinetic control. *Nature*, **1992**, 356, 263-5	50.4	289
592	Optimization of affinity, specificity and function of designed influenza inhibitors using deep sequencing. *Nature Biotechnology*, **2012**, 30, 543-8	44.5	279
591	New algorithms and an in silico benchmark for computational enzyme design. *Protein Science*, **2006**, 15, 2785-94	6.3	278
590	Computational redesign of endonuclease DNA binding and cleavage specificity. *Nature*, **2006**, 441, 656-9	50.4	274
589	Atomic model of the type III secretion system needle. *Nature*, **2012**, 486, 276-9	50.4	270
588	Modeling structurally variable regions in homologous proteins with rosetta. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 656-77	4.2	264
587	Atomic accuracy in predicting and designing noncanonical RNA structure. *Nature Methods*, **2010**, 7, 291-4	21.6	263

586	High-resolution structure prediction and the crystallographic phase problem. *Nature*, **2007**, 450, 259-64	50.4	262
585	Multipass membrane protein structure prediction using Rosetta. *Proteins: Structure, Function and Bioinformatics*, **2006**, 62, 1010-25	4.2	260
584	Important role of hydrogen bonds in the structurally polarized transition state for folding of the src SH3 domain. *Nature Structural and Molecular Biology*, **1998**, 5, 714-20	17.6	256
583	A large scale test of computational protein design: folding and stability of nine completely redesigned globular proteins. *Journal of Molecular Biology*, **2003**, 332, 449-60	6.5	256
582	Computational redesign of protein-protein interaction specificity. *Nature Structural and Molecular Biology*, **2004**, 11, 371-9	17.6	254
581	HMMSTR: a hidden Markov model for local sequence-structure correlations in proteins. *Journal of Molecular Biology*, **2000**, 301, 173-90	6.5	247
580	Atomic-accuracy models from 4.5-Å cryo-electron microscopy data with density-guided iterative local refinement. *Nature Methods*, **2015**, 12, 361-365	21.6	245
579	Functional rapidly folding proteins from simplified amino acid sequences. *Nature Structural Biology*, **1997**, 4, 805-9		245
578	Progress in modeling of protein structures and interactions. *Science*, **2005**, 310, 638-42	33.3	244
577	Design of a hyperstable 60-subunit protein dodecahedron. [corrected]. *Nature*, **2016**, 535, 136-9	50.4	243
576	Global analysis of protein folding using massively parallel design, synthesis, and testing. *Science*, **2017**, 357, 168-175	33.3	241
575	Automated prediction of CASP-5 structures using the Robetta server. *Proteins: Structure, Function and Bioinformatics*, **2003**, 53 Suppl 6, 524-33	4.2	241
574	A synthetic homing endonuclease-based gene drive system in the human malaria mosquito. *Nature*, **2011**, 473, 212-5	50.4	240
573	Assigning function to yeast proteins by integration of technologies. *Molecular Cell*, **2003**, 12, 1353-65	17.6	236
572	Ab initio protein structure prediction: progress and prospects. *Annual Review of Biophysics and Biomolecular Structure*, **2001**, 30, 173-89		236
571	Massively parallel de novo protein design for targeted therapeutics. *Nature*, **2017**, 550, 74-79	50.4	235
570	Accurate de novo design of hyperstable constrained peptides. *Nature*, **2016**, 538, 329-335	50.4	231
569	Refinement of protein structures into low-resolution density maps using rosetta. *Journal of Molecular Biology*, **2009**, 392, 181-90	6.5	230

568	Clustering of low-energy conformations near the native structures of small proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **1998**, 95, 11158-62	11.5	229
567	Elicitation of structure-specific antibodies by epitope scaffolds. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 17880-7	11.5	228
566	Solution structure of a minor and transiently formed state of a T4 lysozyme mutant. *Nature*, **2011**, 477, 111-4	50.4	225
565	De novo enzyme design using Rosetta3. *PLoS ONE*, **2011**, 6, e19230	3.7	224
564	Mechanisms of protein folding. *Current Opinion in Structural Biology*, **2001**, 11, 70-82	8.1	224
563	NMR structure determination for larger proteins using backbone-only data. *Science*, **2010**, 327, 1014-8	33.3	220
562	Kinetics versus thermodynamics in protein folding. *Biochemistry*, **1994**, 33, 7505-9	3.2	219
561	De novo design of picomolar SARS-CoV-2 miniprotein inhibitors. *Science*, **2020**, 370, 426-431	33.3	219
560	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
559	A breakdown of symmetry in the folding transition state of protein L. *Journal of Molecular Biology*, **2000**, 298, 971-84	6.5	210
558	Alternate states of proteins revealed by detailed energy landscape mapping. *Journal of Molecular Biology*, **2011**, 405, 607-18	6.5	207
557	Increased Diels-Alderase activity through backbone remodeling guided by Foldit players. *Nature Biotechnology*, **2012**, 30, 190-2	44.5	206
556	De novo prediction of three-dimensional structures for major protein families. *Journal of Molecular Biology*, **2002**, 322, 65-78	6.5	206
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554	De novo protein structure generation from incomplete chemical shift assignments. *Journal of Biomolecular NMR*, **2009**, 43, 63-78	3	202
553	Design, activity, and structure of a highly specific artificial endonuclease. *Molecular Cell*, **2002**, 10, 895-905	17.6	202
552	RosettaRemodel: a generalized framework for flexible backbone protein design. *PLoS ONE*, **2011**, 6, e24109	3.7	200
551	Computational protein design enables a novel one-carbon assimilation pathway. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 3704-9	11.5	199

550	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
549	High thermodynamic stability of parametrically designed helical bundles. *Science*, **2014**, 346, 481-485	33.3	196
548	Improved molecular replacement by density- and energy-guided protein structure optimization. *Nature*, **2011**, 473, 540-3	50.4	196
547	Voltage sensor conformations in the open and closed states in ROSETTA structural models of K(+) channels. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 7292-7	11.5	196
546	De novo design of protein homo-oligomers with modular hydrogen-bond network-mediated specificity. *Science*, **2016**, 352, 680-7	33.3	194
545	Relaxation of backbone bond geometry improves protein energy landscape modeling. *Protein Science*, **2014**, 23, 47-55	6.3	192
544	Computer-based redesign of a protein folding pathway. *Nature Structural Biology*, **2001**, 8, 602-5		192
543	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
542	Computational redesign of a mononuclear zinc metalloenzyme for organophosphate hydrolysis. *Nature Chemical Biology*, **2012**, 8, 294-300	11.7	189
541	Computational design of protein-protein interactions. *Current Opinion in Chemical Biology*, **2004**, 8, 91-7	9.7	187
540	Evolution of a designed retro-aldolase leads to complete active site remodeling. *Nature Chemical Biology*, **2013**, 9, 494-8	11.7	186
539	Toward high-resolution prediction and design of transmembrane helical protein structures. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 15682-7	11.5	185
538	Engineering an allosteric transcription factor to respond to new ligands. *Nature Methods*, **2016**, 13, 177-83	21.6	184
537	Emergence of a catalytic tetrad during evolution of a highly active artificial aldolase. *Nature Chemistry*, **2017**, 9, 50-56	17.6	184
536	De novo design of potent and selective mimics of IL-2 and IL-15. *Nature*, **2019**, 565, 186-191	50.4	184
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534	GTP-binding Ypt1 protein and Ca2+ function independently in a cell-free protein transport reaction. *Proceedings of the National Academy of Sciences of the United States of America*, **1990**, 87, 355-9	11.5	182
533	A vast repertoire of Dscam binding specificities arises from modular interactions of variable Ig domains. *Cell*, **2007**, 130, 1134-45	56.2	177

532	Structural basis for gating charge movement in the voltage sensor of a sodium channel. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, E93-102	11.5	176
531	Ab initio protein structure prediction of CASP III targets using ROSETTA. *Proteins: Structure, Function and Bioinformatics*, **1999**, Suppl 3, 171-6	4.2	175
530	Bridging the gaps in design methodologies by evolutionary optimization of the stability and proficiency of designed Kemp eliminase KE59. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 10358-63	11.5	174
529	Folding dynamics of the src SH3 domain. *Biochemistry*, **1997**, 36, 15685-92	3.2	174
528	Design of ordered two-dimensional arrays mediated by noncovalent protein-protein interfaces. *Science*, **2015**, 348, 1365-8	33.3	173
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526	Large-scale determination of previously unsolved protein structures using evolutionary information. *ELife*, **2015**, 4, e09248	8.9	173
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524	Evaluation of structural and evolutionary contributions to deleterious mutation prediction. *Journal of Molecular Biology*, **2002**, 322, 891-901	6.5	171
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518	Computationally designed libraries for rapid enzyme stabilization. *Protein Engineering, Design and Selection*, **2014**, 27, 49-58	1.9	164
517	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
516	Structural basis for scaffolding-mediated assembly and maturation of a dsDNA virus. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 1355-60	11.5	162
515	The role of pro regions in protein folding. *Current Opinion in Cell Biology*, **1993**, 5, 966-70	9	160

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513	Exploring the repeat protein universe through computational protein design. *Nature*, **2015**, 528, 580-4	50.4	156
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511	A conserved structural motif mediates formation of the periplasmic rings in the type III secretion system. *Nature Structural and Molecular Biology*, **2009**, 16, 468-76	17.6	154
510	De novo determination of protein backbone structure from residual dipolar couplings using Rosetta. *Journal of the American Chemical Society*, **2002**, 124, 2723-9	16.4	153
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507	Prospects for ab initio protein structural genomics. *Journal of Molecular Biology*, **2001**, 306, 1191-9	6.5	152
506	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
505	Determination of solution structures of proteins up to 40 kDa using CS-Rosetta with sparse NMR data from deuterated samples. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 10873-8	11.5	151
504	Selective targeting of engineered T cells using orthogonal IL-2 cytokine-receptor complexes. *Science*, **2018**, 359, 1037-1042	33.3	149
503	Coupled prediction of protein secondary and tertiary structure. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 12105-10	11.5	148
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500	Prediction of the structure of symmetrical protein assemblies. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 17656-61	11.5	142
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496	An improved protein decoy set for testing energy functions for protein structure prediction. *Proteins: Structure, Function and Bioinformatics*, **2003**, 53, 76-87	4.2	140
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486	De novo protein structure determination from near-atomic-resolution cryo-EM maps. *Nature Methods*, **2015**, 12, 335-8	21.6	131
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473	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
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