Frank DiMaio

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

133 papers	9,474 citations	50 h-index	96 g-index
157 ext. papers	13,663 ext. citations	16.1 avg, IF	6.31 L-index

#	Paper	IF	Citations
133	Structural and functional insight into regulation of kinesin-1 by microtubule-associated protein MAP7.. *Science*, **2022**, 375, 326-331	33.3	8
132	Seipin forms a flexible cage at lipid droplet formation sites.. *Nature Structural and Molecular Biology* , **2022**,	17.6	2
131	Architecture and antigenicity of the Nipah virus attachment glycoprotein.. *Science*, **2022**, eabm5561	33.3	2
130	Large-scale design and refinement of stable proteins using sequence-only models.. *PLoS ONE*, **2022**, 17, e0265020	3.7	0
129	Treponema pallidum genome sequencing from six continents reveals variability in vaccine candidate genes and dominance of Nichols clade strains in Madagascar.. *PLoS Neglected Tropical Diseases*, **2021**, 15, e0010063	4.8	2
128	Cryo-EM structures of CTP synthase filaments reveal mechanism of pH-sensitive assembly during budding yeast starvation. *ELife*, **2021**, 10,	8.9	5
127	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. *Nature Communications*, **2021**, 12, 6947	17.4	0
126	De novo protein design by deep network hallucination. *Nature*, **2021**,	50.4	33
125	Electromechanical coupling mechanism for activation and inactivation of an HCN channel. *Nature Communications*, **2021**, 12, 2802	17.4	4
124	Phospho-regulation, nucleotide binding and ion access control in potassium-chloride cotransporters. *EMBO Journal*, **2021**, 40, e107294	13	5
123	Structure and lipid dynamics in the maintenance of lipid asymmetry inner membrane complex of A. baumannii. *Communications Biology*, **2021**, 4, 817	6.7	4
122	Cryo-electron Microscopy Imaging of Alzheimer's Amyloid-beta 42 Oligomer Displayed on a Functionally and Structurally Relevant Scaffold. *Angewandte Chemie*, **2021**, 133, 18828-18835	3.6	1
121	Cryo-electron Microscopy Imaging of Alzheimer's Amyloid-beta 42 Oligomer Displayed on a Functionally and Structurally Relevant Scaffold. *Angewandte Chemie - International Edition*, **2021**, 60, 18680-18687	16.4	9
120	Perturbing the energy landscape for improved packing during computational protein design. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 436-449	4.2	22
119	Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. *Nature Methods*, **2021**, 18, 156-164	21.6	22
118	BRCA1/BARD1 site-specific ubiquitylation of nucleosomal H2A is directed by BARD1. *Nature Structural and Molecular Biology*, **2021**, 28, 268-277	17.6	21
117	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

116	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
115	Accurate prediction of protein structures and interactions using a three-track neural network. *Science*, **2021**, 373, 871-876	33.3	522
114	Structure of the phosphoinositide 3-kinase (PI3K) p110-p101 complex reveals molecular mechanism of GPCR activation. *Science Advances*, **2021**, 7,	14.3	3
113	Discovery and Characterization of Spike N-Terminal Domain-Binding Aptamers for Rapid SARS-CoV-2 Detection. *Angewandte Chemie*, **2021**, 133, 21381-21385	3.6	1
112	Discovery and Characterization of Spike N-Terminal Domain-Binding Aptamers for Rapid SARS-CoV-2 Detection. *Angewandte Chemie - International Edition*, **2021**, 60, 21211-21215	16.4	9
111	Prediction of Protein Mutational Free Energy: Benchmark and Sampling Improvements Increase Classification Accuracy. *Frontiers in Bioengineering and Biotechnology*, **2020**, 8, 558247	5.8	11
110	Allosteric conformational change of a cyclic nucleotide-gated ion channel revealed by DEER spectroscopy. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 10839-10847	11.5	15
109	Macromolecular modeling and design in Rosetta: recent methods and frameworks. *Nature Methods*, **2020**, 17, 665-680	21.6	165
108	The cryo-EM structure of the bacterial flagellum cap complex suggests a molecular mechanism for filament elongation. *Nature Communications*, **2020**, 11, 3210	17.4	9
107	Polymerization in the actin ATPase clan regulates hexokinase activity in yeast. *Science*, **2020**, 367, 1039-1042	33.3	13
106	Deep learning enables the atomic structure determination of the Fanconi Anemia core complex from cryoEM. *IUCrJ*, **2020**, 7, 881-892	4.7	5
105	Computational design of mixed chirality peptide macrocycles with internal symmetry. *Protein Science*, **2020**, 29, 2433-2445	6.3	9
104	A Structural Model of the Endogenous Human BAF Complex Informs Disease Mechanisms. *Cell*, **2020**, 183, 802-817.e24	56.2	31
103	Efficient consideration of coordinated water molecules improves computational protein-protein and protein-ligand docking discrimination. *PLoS Computational Biology*, **2020**, 16, e1008103	5	19
102	Structural basis for autophagy inhibition by the human Rubicon-Rab7 complex. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 17003-17010	11.5	9
101	Crystal Structure and Mechanistic Molecular Modeling Studies of Diterpene Cyclase Rv3377c. *Biochemistry*, **2020**, 59, 4507-4515	3.2	2
100	Computational design of transmembrane pores. *Nature*, **2020**, 585, 129-134	50.4	56
99	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

98	Processing Structurally Heterogeneous Cryo-EM Data Using Atomic Models. *Microscopy and Microanalysis*, **2019**, 25, 228-229	0.5	
97	Multiple liquid crystalline geometries of highly compacted nucleic acid in a dsRNA virus. *Nature*, **2019**, 570, 252-256	50.4	30
96	Structural basis for substrate gripping and translocation by the ClpB AAA+ disaggregase. *Nature Communications*, **2019**, 10, 2393	17.4	50
95	De novo protein design by citizen scientists. *Nature*, **2019**, 570, 390-394	50.4	63
94	3.1 Å structure of yeast RNA polymerase II elongation complex stalled at a cyclobutane pyrimidine dimer lesion solved using streptavidin affinity grids. *Journal of Structural Biology*, **2019**, 207, 270-278	3.4	12
93	An extensively glycosylated archaeal pilus survives extreme conditions. *Nature Microbiology*, **2019**, 4, 1401-1410	26.6	21
92	Self-Assembling 2D Arrays with de Novo Protein Building Blocks. *Journal of the American Chemical Society*, **2019**, 141, 8891-8895	16.4	24
91	The Molecular Architecture of Native BBSome Obtained by an Integrated Structural Approach. *Structure*, **2019**, 27, 1384-1394.e4	5.2	33
90	The HCN channel voltage sensor undergoes a large downward motion during hyperpolarization. *Nature Structural and Molecular Biology*, **2019**, 26, 686-694	17.6	22
89	COMBINES-CID: An Efficient Method for De Novo Engineering of Highly Specific Chemically Induced Protein Dimerization Systems. *Journal of the American Chemical Society*, **2019**, 141, 10948-10952	16.4	15
88	Structural Studies of Coronavirus Fusion Proteins. *Microscopy and Microanalysis*, **2019**, 25, 1300-1301	0.5	3
87	Phase separation of Polo-like kinase 4 by autoactivation and clustering drives centriole biogenesis. *Nature Communications*, **2019**, 10, 4959	17.4	32
86	Structures of MERS-CoV spike glycoprotein in complex with sialoside attachment receptors. *Nature Structural and Molecular Biology*, **2019**, 26, 1151-1157	17.6	161
85	Programmable design of orthogonal protein heterodimers. *Nature*, **2019**, 565, 106-111	50.4	87
84	Automatically Fixing Errors in Glycoprotein Structures with Rosetta. *Structure*, **2019**, 27, 134-139.e3	5.2	59
83	Cryo-EM structure of the bacterial actin AlfA reveals unique assembly and ATP-binding interactions and the absence of a conserved subdomain. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 3356-3361	11.5	4
82	Accurate computational design of multipass transmembrane proteins. *Science*, **2018**, 359, 1042-1046	33.3	93
81	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

80	Protein structure prediction using Rosetta in CASP12. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86 Suppl 1, 113-121	4.2	63
79	Automatic structure prediction of oligomeric assemblies using Robetta in CASP12. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86 Suppl 1, 283-291	4.2	29
78	Near-atomic model of microtubule-tau interactions. *Science*, **2018**, 360, 1242-1246	33.3	175
77	cryoem-cloud-tools: A software platform to deploy and manage cryo-EM jobs in the cloud. *Journal of Structural Biology*, **2018**, 203, 230-235	3.4	12
76	Germline VRC01 antibody recognition of a modified clade C HIV-1 envelope trimer and a glycosylated HIV-1 gp120 core. *ELife*, **2018**, 7,	8.9	19
75	Structure of the type VI secretion system TssK-TssF-TssG baseplate subcomplex revealed by cryo-electron microscopy. *Nature Communications*, **2018**, 9, 5385	17.4	20
74	Structural Insights into Mdn1, an Essential AAA Protein Required for Ribosome Biogenesis. *Cell*, **2018**, 175, 822-834.e18	56.2	24
73	Cryo-electron microscopy structure of the lipid droplet-formation protein seipin. *Journal of Cell Biology*, **2018**, 217, 4080-4091	7.3	97
72	CryoEM structure of a prokaryotic cyclic nucleotide-gated ion channel. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 4430-4435	11.5	35
71	RosettaES: a sampling strategy enabling automated interpretation of difficult cryo-EM maps. *Nature Methods*, **2017**, 14, 797-800	21.6	84
70	The Therapeutic Antibody LM609 Selectively Inhibits Ligand Binding to Human □Integrin via Steric Hindrance. *Structure*, **2017**, 25, 1732-1739.e5	5.2	20
69	Structural basis of TIR-domain-assembly formation in MAL- and MyD88-dependent TLR4 signaling. *Nature Structural and Molecular Biology*, **2017**, 24, 743-751	17.6	82
68	Structural basis for the initiation of eukaryotic transcription-coupled DNA repair. *Nature*, **2017**, 551, 653-657	50.4	94
67	Cryo-EM structure of the protein-conducting ERAD channel Hrd1 in complex with Hrd3. *Nature*, **2017**, 548, 352-355	50.4	117
66	Modeling oblong proteins and water-mediated interfaces with RosettaDock in CAPRI rounds 28-35. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 479-486	4.2	14
65	Crucial steps in the structure determination of a coronavirus spike glycoprotein using cryo-electron microscopy. *Protein Science*, **2017**, 26, 113-121	6.3	28
64	Anti-diabetic drug binding site in a mammalian K channel revealed by Cryo-EM. *ELife*, **2017**, 6,	8.9	81
63	Model for a novel membrane envelope in a filamentous hyperthermophilic virus. *ELife*, **2017**, 6,	8.9	32

62	Rosetta Structure Prediction as a Tool for Solving Difficult Molecular Replacement Problems. *Methods in Molecular Biology*, **2017**, 1607, 455-466	1.4	6
61	Glycan shield and epitope masking of a coronavirus spike protein observed by cryo-electron microscopy. *Nature Structural and Molecular Biology*, **2016**, 23, 899-905	17.6	252
60	Cryo-EM Structure of Caspase-8 Tandem DED Filament Reveals Assembly and Regulation Mechanisms of the Death-Inducing Signaling Complex. *Molecular Cell*, **2016**, 64, 236-250	17.6	89
59	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
58	Structure of a Chaperone-Usher Pilus Reveals the Molecular Basis of Rod Uncoiling. *Cell*, **2016**, 164, 269-278	56.2	41
57	Cryo-electron microscopy structure of a coronavirus spike glycoprotein trimer. *Nature*, **2016**, 531, 114-117	50.4	354
56	Automated structure refinement of macromolecular assemblies from cryo-EM maps using Rosetta. *ELife*, **2016**, 5,	8.9	227
55	Author response: Automated structure refinement of macromolecular assemblies from cryo-EM maps using Rosetta **2016**,		5
54	Tools for Model Building and Optimization into Near-Atomic Resolution Electron Cryo-Microscopy Density Maps. *Methods in Enzymology*, **2016**, 579, 255-76	1.7	23
53	Improving hybrid statistical and physical forcefields through local structure enumeration. *Protein Science*, **2016**, 25, 1525-34	6.3	5
52	CASP11 refinement experiments with ROSETTA. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84 Suppl 1, 314-22	4.2	18
51	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
50	De novo design of protein homo-oligomers with modular hydrogen-bond network-mediated specificity. *Science*, **2016**, 352, 680-7	33.3	194
49	Protocols for Molecular Modeling with Rosetta3 and RosettaScripts. *Biochemistry*, **2016**, 55, 4748-63	3.2	118
48	Structure of the type VI secretion system contractile sheath. *Cell*, **2015**, 160, 952-962	56.2	172
47	De novo protein structure determination from near-atomic-resolution cryo-EM maps. *Nature Methods*, **2015**, 12, 335-8	21.6	131
46	Designing Two-Dimensional Protein Arrays through Fusion of Multimers and Interface Mutations. *Nano Letters*, **2015**, 15, 5235-9	11.5	35
45	The molecular basis for flexibility in the flexible filamentous plant viruses. *Nature Structural and Molecular Biology*, **2015**, 22, 642-4	17.6	45

44	Unique double-ring structure of the peroxisomal Pex1/Pex6 ATPase complex revealed by cryo-electron microscopy. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E4017-25	11.5	50
43	Design of ordered two-dimensional arrays mediated by noncovalent protein-protein interfaces. *Science*, **2015**, 348, 1365-8	33.3	173
42	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
41	EMRinger: side chain-directed model and map validation for 3D cryo-electron microscopy. *Nature Methods*, **2015**, 12, 943-6	21.6	523
40	Virology. A virus that infects a hyperthermophile encapsidates A-form DNA. *Science*, **2015**, 348, 914-7	33.3	79
39	The origin of consistent protein structure refinement from structural averaging. *Structure*, **2015**, 23, 1123-8	5.2	14
38	Structure of EspB from the ESX-1 type VII secretion system and insights into its export mechanism. *Structure*, **2015**, 23, 571-583	5.2	57
37	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
36	One contact for every twelve residues allows robust and accurate topology-level protein structure modeling. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82 Suppl 2, 208-18	4.2	70
35	Relaxation of backbone bond geometry improves protein energy landscape modeling. *Protein Science*, **2014**, 23, 47-55	6.3	192
34	Crystal structure of the transport unit of the autotransporter adhesin involved in diffuse adherence from Escherichia coli. *Journal of Structural Biology*, **2014**, 187, 20-29	3.4	26
33	High thermodynamic stability of parametrically designed helical bundles. *Science*, **2014**, 346, 481-485	33.3	196
32	Crystal structure analysis of EstA from Arthrobacter sp. Rue61a--an insight into catalytic promiscuity. *FEBS Letters*, **2014**, 588, 1154-60	3.8	13
31	Improved low-resolution crystallographic refinement with Phenix and Rosetta. *Nature Methods*, **2013**, 10, 1102-4	21.6	137
30	High-resolution comparative modeling with RosettaCM. *Structure*, **2013**, 21, 1735-42	5.2	649
29	Advances, interactions, and future developments in the CNS, Phenix, and Rosetta structural biology software systems. *Annual Review of Biophysics*, **2013**, 42, 265-87	21.1	76
28	Cryo-EM model validation using independent map reconstructions. *Protein Science*, **2013**, 22, 865-8	6.3	64
27	Protein Structure Modeling with Rosetta: Case Studies in Structure Prediction and Enzyme Repurposing. *NATO Science for Peace and Security Series A: Chemistry and Biology*, **2013**, 353-362	0.1	

26	Structure of the C-terminal region of an ERG channel and functional implications. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 11648-53	11.5	50
25	A refined model of the prototypical Salmonella SPI-1 T3SS basal body reveals the molecular basis for its assembly. *PLoS Pathogens*, **2013**, 9, e1003307	7.6	63
24	Advances in Rosetta structure prediction for difficult molecular-replacement problems. *Acta Crystallographica Section D: Biological Crystallography*, **2013**, 69, 2202-8		18
23	The dynamic disulphide relay of quiescin sulphydryl oxidase. *Nature*, **2012**, 488, 414-8	50.4	62
22	phenix.mr_rosetta: molecular replacement and model rebuilding with Phenix and Rosetta. *Journal of Structural and Functional Genomics*, **2012**, 13, 81-90		109
21	Structure and stoichiometry of an accessory subunit TRIP8b interaction with hyperpolarization-activated cyclic nucleotide-gated channels. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 7899-904	11.5	40
20	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
19	Alternate states of proteins revealed by detailed energy landscape mapping. *Journal of Molecular Biology*, **2011**, 405, 607-18	6.5	207
18	Crystal structure of XMRV protease differs from the structures of other retropepsins. *Nature Structural and Molecular Biology*, **2011**, 18, 227-9	17.6	26
17	Improved molecular replacement by density- and energy-guided protein structure optimization. *Nature*, **2011**, 473, 540-3	50.4	196
16	Cryo-EM structure of a group II chaperonin in the prehydrolysis ATP-bound state leading to lid closure. *Structure*, **2011**, 19, 633-9	5.2	45
15	High-resolution structure of a retroviral protease folded as a monomer. *Acta Crystallographica Section D: Biological Crystallography*, **2011**, 67, 907-14		15
14	Determination of the structures of symmetric protein oligomers from NMR chemical shifts and residual dipolar couplings. *Journal of the American Chemical Society*, **2011**, 133, 6288-98	16.4	55
13	Crystal structure of Toll-like receptor adaptor MAL/TIRAP reveals the molecular basis for signal transduction and disease protection. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 14879-84	11.5	105
12	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
11	Modeling symmetric macromolecular structures in Rosetta3. *PLoS ONE*, **2011**, 6, e20450	3.7	142
10	Analyses of subnanometer resolution cryo-EM density maps. *Methods in Enzymology*, **2010**, 483, 1-29	1.7	20
9	Refinement of protein structures into low-resolution density maps using rosetta. *Journal of Molecular Biology*, **2009**, 392, 181-90	6.5	230

8	Spherical-harmonic decomposition for molecular recognition in electron-density maps. *International Journal of Data Mining and Bioinformatics*, **2009**, 3, 205-27	0.5	4
7	Independent evolution of polymerization in the Actin ATPase clan regulates hexokinase activity		1
6	Prediction of protein mutational free energy: benchmark and sampling improvements increase classification accuracy		1
5	Deep learning enables the atomic structure determination of the Fanconi Anemia core complex from cryoEM		1
4	Atomic model of microtubule-bound tau		3
3	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks		2
2	Cryo-EM Structures of CTP Synthase Filaments Reveal Mechanism of pH-Sensitive Assembly During Budding Yeast Starvation		1
1	Growing Glycans in Rosetta: Accurate de novo glycan modeling, density fitting, and rational sequon design		2