

Frank DiMaio

List of Publications by Year in descending order

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Version: 2024-02-01

132
papers

16,917
citations

26626

56
h-index

20358

116
g-index

157
all docs

157
docs citations

157
times ranked

19804
citing authors

#	ARTICLE	IF	CITATIONS
1	Accurate prediction of protein structures and interactions using a three-track neural network. <i>Science</i> , 2021, 373, 871-876.	12.6	2,843
2	High-Resolution Comparative Modeling with RosettaCM. <i>Structure</i> , 2013, 21, 1735-1742.	3.3	1,010
3	EMRinger: side chain-directed model and map validation for 3D cryo-electron microscopy. <i>Nature Methods</i> , 2015, 12, 943-946.	19.0	799
4	Macromolecular modeling and design in Rosetta: recent methods and frameworks. <i>Nature Methods</i> , 2020, 17, 665-680.	19.0	513
5	Crystal structure of a monomeric retroviral protease solved by protein folding game players. <i>Nature Structural and Molecular Biology</i> , 2011, 18, 1175-1177.	8.2	463
6	Cryo-electron microscopy structure of a coronavirus spike glycoprotein trimer. <i>Nature</i> , 2016, 531, 114-117.	27.8	453
7	Automated structure refinement of macromolecular assemblies from cryo-EM maps using Rosetta. <i>ELife</i> , 2016, 5, .	6.0	407
8	Simultaneous Optimization of Biomolecular Energy Functions on Features from Small Molecules and Macromolecules. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 6201-6212.	5.3	382
9	Glycan shield and epitope masking of a coronavirus spike protein observed by cryo-electron microscopy. <i>Nature Structural and Molecular Biology</i> , 2016, 23, 899-905.	8.2	366
10	Alternate States of Proteins Revealed by Detailed Energy Landscape Mapping. <i>Journal of Molecular Biology</i> , 2011, 405, 607-618.	4.2	324
11	Relaxation of backbone bond geometry improves protein energy landscape modeling. <i>Protein Science</i> , 2014, 23, 47-55.	7.6	323
12	Atomic-accuracy models from 4.5-Å... cryo-electron microscopy data with density-guided iterative local refinement. <i>Nature Methods</i> , 2015, 12, 361-365.	19.0	313
13	Near-atomic model of microtubule-tau interactions. <i>Science</i> , 2018, 360, 1242-1246.	12.6	285
14	De novo protein design by deep network hallucination. <i>Nature</i> , 2021, 600, 547-552.	27.8	280
15	Refinement of Protein Structures into Low-Resolution Density Maps Using Rosetta. <i>Journal of Molecular Biology</i> , 2009, 392, 181-190.	4.2	272
16	High thermodynamic stability of parametrically designed helical bundles. <i>Science</i> , 2014, 346, 481-485.	12.6	264
17	De novo design of protein homo-oligomers with modular hydrogen-bond network-mediated specificity. <i>Science</i> , 2016, 352, 680-687.	12.6	262
18	Improved molecular replacement by density- and energy-guided protein structure optimization. <i>Nature</i> , 2011, 473, 540-543.	27.8	226

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19	Design of ordered two-dimensional arrays mediated by noncovalent protein-protein interfaces. <i>Science</i> , 2015, 348, 1365-1368.	12.6	219
20	Structures of MERS-CoV spike glycoprotein in complex with sialoside attachment receptors. <i>Nature Structural and Molecular Biology</i> , 2019, 26, 1151-1157.	8.2	218
21	Structure of the Type VI Secretion System Contractile Sheath. <i>Cell</i> , 2015, 160, 952-962.	28.9	216
22	Combined Covalent-Electrostatic Model of Hydrogen Bonding Improves Structure Prediction with Rosetta. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 609-622.	5.3	204
23	Modeling Symmetric Macromolecular Structures in Rosetta3. <i>PLoS ONE</i> , 2011, 6, e20450.	2.5	197
24	Structural basis for scaffolding-mediated assembly and maturation of a dsDNA virus. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 1355-1360.	7.1	191
25	Protocols for Molecular Modeling with Rosetta3 and RosettaScripts. <i>Biochemistry</i> , 2016, 55, 4748-4763.	2.5	182
26	Improved low-resolution crystallographic refinement with Phenix and Rosetta. <i>Nature Methods</i> , 2013, 10, 1102-1104.	19.0	175
27	De novo protein structure determination from near-atomic-resolution cryo-EM maps. <i>Nature Methods</i> , 2015, 12, 335-338.	19.0	172
28	Cryo-EM structure of the protein-conducting ERAD channel Hrd1 in complex with Hrd3. <i>Nature</i> , 2017, 548, 352-355.	27.8	160
29	Structural basis for the initiation of eukaryotic transcription-coupled DNA repair. <i>Nature</i> , 2017, 551, 653-657.	27.8	151
30	Accurate computational design of multipass transmembrane proteins. <i>Science</i> , 2018, 359, 1042-1046.	12.6	149
31	Cryo-electron microscopy structure of the lipid droplet formation protein seipin. <i>Journal of Cell Biology</i> , 2018, 217, 4080-4091.	5.2	147
32	Structural basis of TIR-domain-assembly formation in MAL- and MyD88-dependent TLR4 signaling. <i>Nature Structural and Molecular Biology</i> , 2017, 24, 743-751.	8.2	140
33	Programmable design of orthogonal protein heterodimers. <i>Nature</i> , 2019, 565, 106-111.	27.8	139
34	phenix.mr_rosetta: molecular replacement and model rebuilding with Phenix and Rosetta. <i>Journal of Structural and Functional Genomics</i> , 2012, 13, 81-90.	1.2	131
35	Cryo-EM Structure of Caspase-8 Tandem DED Filament Reveals Assembly and Regulation Mechanisms of the Death-Inducing Signaling Complex. <i>Molecular Cell</i> , 2016, 64, 236-250.	9.7	128
36	Crystal structure of Toll-like receptor adaptor MAL/TIRAP reveals the molecular basis for signal transduction and disease protection. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 14879-14884.	7.1	123

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37	Anti-diabetic drug binding site in a mammalian KATP channel revealed by Cryo-EM. <i>ELife</i> , 2017, 6, .	6.0	122
38	Computational design of transmembrane pores. <i>Nature</i> , 2020, 585, 129-134.	27.8	120
39	RosettaES: a sampling strategy enabling automated interpretation of difficult cryo-EM maps. <i>Nature Methods</i> , 2017, 14, 797-800.	19.0	118
40	De novo protein design by citizen scientists. <i>Nature</i> , 2019, 570, 390-394.	27.8	105
41	A Structural Model of the Endogenous Human BAF Complex Informs Disease Mechanisms. <i>Cell</i> , 2020, 183, 802-817.e24.	28.9	100
42	A virus that infects a hyperthermophile encapsidates A-form DNA. <i>Science</i> , 2015, 348, 914-917.	12.6	98
43	Improved de novo structure prediction in <scp>CASP</scp> 11 by incorporating coevolution information into Rosetta. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 67-75.	2.6	96
44	Automatically Fixing Errors in Glycoprotein Structures with Rosetta. <i>Structure</i> , 2019, 27, 134-139.e3.	3.3	93
45	Advances, Interactions, and Future Developments in the CNS, Phenix, and Rosetta Structural Biology Software Systems. <i>Annual Review of Biophysics</i> , 2013, 42, 265-287.	10.0	88
46	Structural basis for substrate gripping and translocation by the ClpB AAA+ disaggregase. <i>Nature Communications</i> , 2019, 10, 2393.	12.8	88
47	One contact for every twelve residues allows robust and accurate topology-level protein structure modeling. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 208-218.	2.6	87
48	Structure of EspB from the ESX-1 Type VII Secretion System and Insights into its Export Mechanism. <i>Structure</i> , 2015, 23, 571-583.	3.3	85
49	Protein structure prediction using Rosetta in CASP12. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 113-121.	2.6	85
50	Perturbing the energy landscape for improved packing during computational protein design. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 436-449.	2.6	85
51	A Refined Model of the Prototypical Salmonella SPI-1 T3SS Basal Body Reveals the Molecular Basis for Its Assembly. <i>PLoS Pathogens</i> , 2013, 9, e1003307.	4.7	76
52	Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. <i>Nature Methods</i> , 2021, 18, 156-164.	19.0	73
53	Cryo-EM model validation using independent map reconstructions. <i>Protein Science</i> , 2013, 22, 865-868.	7.6	72
54	The molecular basis for flexibility in the flexible filamentous plant viruses. <i>Nature Structural and Molecular Biology</i> , 2015, 22, 642-644.	8.2	72

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55	Unique double-ring structure of the peroxisomal Pex1/Pex6 ATPase complex revealed by cryo-electron microscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E4017-25.	7.1	72
56	The dynamic disulphide relay of quiescin sulphhydryl oxidase. <i>Nature</i> , 2012, 488, 414-418.	27.8	70
57	Determination of the Structures of Symmetric Protein Oligomers from NMR Chemical Shifts and Residual Dipolar Couplings. <i>Journal of the American Chemical Society</i> , 2011, 133, 6288-6298.	13.7	65
58	Protein homology model refinement by large-scale energy optimization. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 3054-3059.	7.1	62
59	An enumerative algorithm for de novo design of proteins with diverse pocket structures. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 22135-22145.	7.1	62
60	Discovery and Characterization of Spike N-Terminal Domain-Binding Aptamers for Rapid SARS-CoV-2 Detection. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 21211-21215.	13.8	62
61	Structure of a Chaperone-Usher Pilus Reveals the Molecular Basis of Rod Uncoiling. <i>Cell</i> , 2016, 164, 269-278.	28.9	61
62	Structure of the C-terminal region of an ERG channel and functional implications. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 11648-11653.	7.1	59
63	Multiple liquid crystalline geometries of highly compacted nucleic acid in a dsRNA virus. <i>Nature</i> , 2019, 570, 252-256.	27.8	59
64	BRCA1/BARD1 site-specific ubiquitylation of nucleosomal H2A is directed by BARD1. <i>Nature Structural and Molecular Biology</i> , 2021, 28, 268-277.	8.2	58
65	Phase separation of Polo-like kinase 4 by autoactivation and clustering drives centriole biogenesis. <i>Nature Communications</i> , 2019, 10, 4959.	12.8	55
66	Prediction of Protein Mutational Free Energy: Benchmark and Sampling Improvements Increase Classification Accuracy. <i>Frontiers in Bioengineering and Biotechnology</i> , 2020, 8, 558247.	4.1	55
67	Structural and functional insight into regulation of kinesin-1 by microtubule-associated protein MAP7. <i>Science</i> , 2022, 375, 326-331.	12.6	53
68	Cryo-EM Structure of a Group II Chaperonin in the Prehydrolysis ATP-Bound State Leading to Lid Closure. <i>Structure</i> , 2011, 19, 633-639.	3.3	52
69	The HCN channel voltage sensor undergoes a large downward motion during hyperpolarization. <i>Nature Structural and Molecular Biology</i> , 2019, 26, 686-694.	8.2	52
70	Force Field Optimization Guided by Small Molecule Crystal Lattice Data Enables Consistent Sub-Angstrom Protein-Ligand Docking. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2000-2010.	5.3	52
71	Structure and stoichiometry of an accessory subunit TRIP8b interaction with hyperpolarization-activated cyclic nucleotide-gated channels. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 7899-7904.	7.1	51
72	CryoEM structure of a prokaryotic cyclic nucleotide-gated ion channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 4430-4435.	7.1	51

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73	The Molecular Architecture of Native BBSome Obtained by an Integrated Structural Approach. <i>Structure</i> , 2019, 27, 1384-1394.e4.	3.3	51
74	Automatic structure prediction of oligomeric assemblies using Robetta in CASP12. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 283-291.	2.6	49
75	An extensively glycosylated archaeal pilus survives extreme conditions. <i>Nature Microbiology</i> , 2019, 4, 1401-1410.	13.3	46
76	Structural Insights into Mdn1, an Essential AAA Protein Required for Ribosome Biogenesis. <i>Cell</i> , 2018, 175, 822-834.e18.	28.9	42
77	Polymerization in the actin ATPase clan regulates hexokinase activity in yeast. <i>Science</i> , 2020, 367, 1039-1042.	12.6	41
78	Efficient consideration of coordinated water molecules improves computational protein-protein and protein-ligand docking discrimination. <i>PLoS Computational Biology</i> , 2020, 16, e1008103.	3.2	39
79	Cryo-electron Microscopy Imaging of Alzheimer's Amyloid β 42 Oligomer Displayed on a Functionally and Structurally Relevant Scaffold. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 18680-18687.	13.8	39
80	Designing Two-Dimensional Protein Arrays through Fusion of Multimers and Interface Mutations. <i>Nano Letters</i> , 2015, 15, 5235-5239.	9.1	38
81	Allosteric conformational change of a cyclic nucleotide-gated ion channel revealed by DEER spectroscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 10839-10847.	7.1	38
82	Structure of the type VI secretion system TssK-TssF-TssG baseplate subcomplex revealed by cryo-electron microscopy. <i>Nature Communications</i> , 2018, 9, 5385.	12.8	37
83	Self-Assembling 2D Arrays with <i>de Novo</i> Protein Building Blocks. <i>Journal of the American Chemical Society</i> , 2019, 141, 8891-8895.	13.7	37
84	Model for a novel membrane envelope in a filamentous hyperthermophilic virus. <i>ELife</i> , 2017, 6, .	6.0	37
85	COMBINES-CID: An Efficient Method for De Novo Engineering of Highly Specific Chemically Induced Protein Dimerization Systems. <i>Journal of the American Chemical Society</i> , 2019, 141, 10948-10952.	13.7	34
86	Seipin forms a flexible cage at lipid droplet formation sites. <i>Nature Structural and Molecular Biology</i> , 2022, 29, 194-202.	8.2	33
87	Architecture and antigenicity of the Nipah virus attachment glycoprotein. <i>Science</i> , 2022, 375, 1373-1378.	12.6	33
88	Germline VRC01 antibody recognition of a modified clade C HIV-1 envelope trimer and a glycosylated HIV-1 gp120 core. <i>ELife</i> , 2018, 7, .	6.0	32
89	Crucial steps in the structure determination of a coronavirus spike glycoprotein using cryo-electron microscopy. <i>Protein Science</i> , 2017, 26, 113-121.	7.6	31
90	Structure and lipid dynamics in the maintenance of lipid asymmetry inner membrane complex of <i>A. baumannii</i> . <i>Communications Biology</i> , 2021, 4, 817.	4.4	31

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91	Crystal structure of the transport unit of the autotransporter adhesin involved in diffuse adherence from <i>Escherichia coli</i> . <i>Journal of Structural Biology</i> , 2014, 187, 20-29.	2.8	30
92	<i>Treponema pallidum</i> genome sequencing from six continents reveals variability in vaccine candidate genes and dominance of Nichols clade strains in Madagascar. <i>PLoS Neglected Tropical Diseases</i> , 2021, 15, e0010063.	3.0	30
93	Tools for Model Building and Optimization into Near-Atomic Resolution Electron Cryo-Microscopy Density Maps. <i>Methods in Enzymology</i> , 2016, 579, 255-276.	1.0	28
94	Computational design of a synthetic PD-1 agonist. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	28
95	Crystal structure of XMRV protease differs from the structures of other retropepsins. <i>Nature Structural and Molecular Biology</i> , 2011, 18, 227-229.	8.2	27
96	3.1 Å structure of yeast RNA polymerase II elongation complex stalled at a cyclobutane pyrimidine dimer lesion solved using streptavidin affinity grids. <i>Journal of Structural Biology</i> , 2019, 207, 270-278.	2.8	27
97	CASP 11 refinement experiments with ROSETTA. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 314-322.	2.6	26
98	Structure of the phosphoinositide 3-kinase (PI3K) p110 ^β -p101 complex reveals molecular mechanism of GPCR activation. <i>Science Advances</i> , 2021, 7, .	10.3	25
99	Cryo-EM structures of CTP synthase filaments reveal mechanism of pH-sensitive assembly during budding yeast starvation. <i>ELife</i> , 2021, 10, .	6.0	25
100	The Therapeutic Antibody LM609 Selectively Inhibits Ligand Binding to Human α 2 β 3 Integrin via Steric Hindrance. <i>Structure</i> , 2017, 25, 1732-1739.e5.	3.3	24
101	Analyses of Subnanometer Resolution Cryo-EM Density Maps. <i>Methods in Enzymology</i> , 2010, 483, 1-29.	1.0	22
102	High-resolution structure of a retroviral protease folded as a monomer. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011, 67, 907-914.	2.5	22
103	Advances in Rosetta structure prediction for difficult molecular-replacement problems. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 2202-2208.	2.5	20
104	cryoem-cloud-tools: A software platform to deploy and manage cryo-EM jobs in the cloud. <i>Journal of Structural Biology</i> , 2018, 203, 230-235.	2.8	19
105	Phosphoregulation, nucleotide binding and ion access control in potassium-chloride cotransporters. <i>EMBO Journal</i> , 2021, 40, e107294.	7.8	19
106	Modeling oblong proteins and water-mediated interfaces with RosettaDock in CAPRI rounds 28-35. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 479-486.	2.6	18
107	Structural basis for autophagy inhibition by the human Rubicon-Rab7 complex. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 17003-17010.	7.1	18
108	Electromechanical coupling mechanism for activation and inactivation of an HCN channel. <i>Nature Communications</i> , 2021, 12, 2802.	12.8	17

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109	Large-scale design and refinement of stable proteins using sequence-only models. PLoS ONE, 2022, 17, e0265020.	2.5	17
110	The Origin of Consistent Protein Structure Refinement from Structural Averaging. Structure, 2015, 23, 1123-1128.	3.3	16
111	Computational design of mixed chirality peptide macrocycles with internal symmetry. Protein Science, 2020, 29, 2433-2445.	7.6	16
112	The cryo-EM structure of the bacterial flagellum cap complex suggests a molecular mechanism for filament elongation. Nature Communications, 2020, 11, 3210.	12.8	16
113	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Nature Communications, 2021, 12, 6947.	12.8	16
114	Crystal structure analysis of EstA from <i>Arthrobacter</i> sp. Rue61a – an insight into catalytic promiscuity. FEBS Letters, 2014, 588, 1154-1160.	2.8	14
115	Discovery and Characterization of Spike N-Terminal Domain-Binding Aptamers for Rapid SARS-CoV-2 Detection. Angewandte Chemie, 2021, 133, 21381-21385.	2.0	14
116	Rosetta Structure Prediction as a Tool for Solving Difficult Molecular Replacement Problems. Methods in Molecular Biology, 2017, 1607, 455-466.	0.9	11
117	Deep learning enables the atomic structure determination of the Fanconi Anemia core complex from cryoEM. IUCr, 2020, 7, 881-892.	2.2	10
118	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.	7.1	7
119	Spherical-harmonic decomposition for molecular recognition in electron-density maps. International Journal of Data Mining and Bioinformatics, 2009, 3, 205.	0.1	6
120	Improving hybrid statistical and physical forcefields through local structure enumeration. Protein Science, 2016, 25, 1525-1534.	7.6	6
121	Crystal Structure and Mechanistic Molecular Modeling Studies of Mycobacterium tuberculosis Diterpene Cyclase Rv3377c. Biochemistry, 2020, 59, 4507-4515.	2.5	6
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.	2.0	5
123	Structural Studies of Coronavirus Fusion Proteins. Microscopy and Microanalysis, 2019, 25, 1300-1301.	0.4	4
124	Suppressor Mutations in Type II Secretion Mutants of <i>Vibrio cholerae</i> : Inactivation of the VesC Protease. MSphere, 2020, 5, .	2.9	2
125	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.	0.5	0
126	Processing Structurally Heterogeneous Cryo-EM Data Using Atomic Models. Microscopy and Microanalysis, 2019, 25, 228-229.	0.4	0

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127	Title is missing!. , 2020, 16, e1008103.		0
128	Title is missing!. , 2020, 16, e1008103.		0
129	Title is missing!. , 2020, 16, e1008103.		0
130	Title is missing!. , 2020, 16, e1008103.		0
131	Title is missing!. , 2020, 16, e1008103.		0
132	Title is missing!. , 2020, 16, e1008103.		0