Frank DiMaio

List of Publications by Year
in descending order

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132 papers	16,917 citations	26630 56 h-index	20358 116 g-index
157 all docs	157 docs citations	157 times ranked	19804 citing authors

#	Article	IF	Citations
1	Structural and functional insight into regulation of kinesin-1 by microtubule-associated protein MAP7. Science, 2022, 375, 326-331.	12.6	53
2	Seipin forms a flexible cage at lipid droplet formation sites. Nature Structural and Molecular Biology, 2022, 29, 194-202.	8.2	33
3	Architecture and antigenicity of the Nipah virus attachment glycoprotein. Science, 2022, 375, 1373-1378.	12.6	33
4	Large-scale design and refinement of stable proteins using sequence-only models. PLoS ONE, 2022, 17, e0265020.	2.5	17
5	Perturbing the energy landscape for improved packing during computational protein design. Proteins: Structure, Function and Bioinformatics, 2021, 89, 436-449.	2.6	85
6	Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. Nature Methods, 2021, 18, 156-164.	19.0	73
7	BRCA1/BARD1 site-specific ubiquitylation of nucleosomal H2A is directed by BARD1. Nature Structural and Molecular Biology, 2021, 28, 268-277.	8.2	58
8	Force Field Optimization Guided by Small Molecule Crystal Lattice Data Enables Consistent Sub-Angstrom Proteinâ€“Ligand Docking. Journal of Chemical Theory and Computation, 2021, 17, 2000-2010.	5.3	52
9	Electromechanical coupling mechanism for activation and inactivation of an HCN channel. Nature Communications, 2021, 12, 2802.	12.8	17
10	Phosphoâ€regulation, nucleotide binding and ion access control in potassiumâ€chloride cotransporters. EMBO Journal, 2021, 40, e107294.	7.8	19
11	Structure and lipid dynamics in the maintenance of lipid asymmetry inner membrane complex of A. baumannii. Communications Biology, 2021, 4, 817.	4.4	31
12	Cryoâ€electron Microscopy Imaging of Alzheimer's Amyloidâ€beta 42 Oligomer Displayed on a Functionally and Structurally Relevant Scaffold. Angewandte Chemie, 2021, 133, 18828-18835.	2.0	5
13	Cryoâ€electron Microscopy Imaging of Alzheimer's Amyloidâ€beta 42 Oligomer Displayed on a Functionally and Structurally Relevant Scaffold. Angewandte Chemie - International Edition, 2021, 60, 18680-18687.	13.8	39
14	Computational design of a synthetic PD-1 agonist. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	28
15	Accurate prediction of protein structures and interactions using a three-track neural network. Science, 2021, 373, 871-876.	12.6	2,843
16	Structure of the phosphoinositide 3-kinase (PI3K) p110Î³-p101 complex reveals molecular mechanism of GPCR activation. Science Advances, 2021, 7, .	10.3	25
17	Discovery and Characterization of Spike Nâ€Terminal Domainâ€Binding Aptamers for Rapid SARSâ€CoVâ€2 Detection. Angewandte Chemie, 2021, 133, 21381-21385.	2.0	14
18	Discovery and Characterization of Spike Nâ€Terminal Domainâ€Binding Aptamers for Rapid SARSâ€CoVâ€2 Detection. Angewandte Chemie - International Edition, 2021, 60, 21211-21215.	13.8	62

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19	Cryo-EM structures of CTP synthase filaments reveal mechanism of pH-sensitive assembly during budding yeast starvation. ELife, 2021, 10, .	6.0	25
20	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Nature Communications, 2021, 12, 6947.	12.8	16
21	De novo protein design by deep network hallucination. Nature, 2021, 600, 547-552.	27.8	280
22	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.	3.0	30
23	Computational design of mixed chirality peptide macrocycles with internal symmetry. Protein Science, 2020, 29, 2433-2445.	7.6	16
24	A Structural Model of the Endogenous Human BAF Complex Informs Disease Mechanisms. Cell, 2020, 183, 802-817.e24.	28.9	100
25	Efficient consideration of coordinated water molecules improves computational protein-protein and protein-ligand docking discrimination. PLoS Computational Biology, 2020, 16, e1008103.	3.2	39
26	Structural basis for autophagy inhibition by the human Rubiconâ€“Rab7 complex. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 17003-17010.	7.1	18
27	Crystal Structure and Mechanistic Molecular Modeling Studies ofMycobacterium tuberculosisDiterpene Cyclase Rv3377c. Biochemistry, 2020, 59, 4507-4515.	2.5	6
28	Computational design of transmembrane pores. Nature, 2020, 585, 129-134.	27.8	120
29	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.	7.1	62
30	Prediction of Protein Mutational Free Energy: Benchmark and Sampling Improvements Increase Classification Accuracy. Frontiers in Bioengineering and Biotechnology, 2020, 8, 558247.	4.1	55
31	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.	7.1	38
32	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	19.0	513
33	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
34	Polymerization in the actin ATPase clan regulates hexokinase activity in yeast. Science, 2020, 367, 1039-1042.	12.6	41
35	Deep learning enables the atomic structure determination of the Fanconi Anemia core complex from cryoEM. IUCrJ, 2020, 7, 881-892.	2.2	10
36	Suppressor Mutations in Type II Secretion Mutants of Vibrio cholerae: Inactivation of the VesC Protease. MSphere, 2020, 5, .	2.9	2

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37	Title is missing!. , 2020, 16, e1008103.		0
38	Title is missing!. , 2020, 16, e1008103.		0
39	Title is missing!. , 2020, 16, e1008103.		0
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41	Title is missing!. , 2020, 16, e1008103.		0
42	Title is missing!. , 2020, 16, e1008103.		0
43	The Molecular Architecture of Native BBSome Obtained by an Integrated Structural Approach. Structure, 2019, 27, 1384-1394.e4.	3.3	51
44	The HCN channel voltage sensor undergoes a large downward motion during hyperpolarization. Nature Structural and Molecular Biology, 2019, 26, 686-694.	8.2	52
45	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.	13.7	34
46	Structural Studies of Coronavirus Fusion Proteins. Microscopy and Microanalysis, 2019, 25, 1300-1301.	0.4	4
47	Phase separation of Polo-like kinase 4 by autoactivation and clustering drives centriole biogenesis. Nature Communications, 2019, 10, 4959.	12.8	55
48	Processing Structurally Heterogeneous Cryo-EM Data Using Atomic Models. Microscopy and Microanalysis, 2019, 25, 228-229.	0.4	0
49	Multiple liquid crystalline geometries of highly compacted nucleic acid in a dsRNA virus. Nature, 2019, 570, 252-256.	27.8	59
50	Structural basis for substrate gripping and translocation by the ClpB AAA+ disaggregase. Nature Communications, 2019, 10, 2393.	12.8	88
51	De novo protein design by citizen scientists. Nature, 2019, 570, 390-394.	27.8	105
52	3.1â€Ã… 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.	2.8	27
53	An extensively glycosylated archaeal pilus survives extreme conditions. Nature Microbiology, 2019, 4, 1401-1410.	13.3	46
54	Self-Assembling 2D Arrays with de Novo Protein Building Blocks. Journal of the American Chemical Society, 2019, 141, 8891-8895.	13.7	37

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55	Structures of MERS-CoV spike glycoprotein in complex with sialoside attachment receptors. Nature Structural and Molecular Biology, 2019, 26, 1151-1157.	8.2	218
56	Programmable design of orthogonal protein heterodimers. Nature, 2019, 565, 106-111.	27.8	139
57	Automatically Fixing Errors in Glycoprotein Structures with Rosetta. Structure, 2019, 27, 134-139.e3.	3.3	93
58	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
59	Accurate computational design of multipass transmembrane proteins. Science, 2018, 359, 1042-1046.	12.6	149
60	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.	7.1	62
61	Protein structure prediction using Rosetta in CASP12. Proteins: Structure, Function and Bioinformatics, 2018, 86, 113-121.	2.6	85
62	Automatic structure prediction of oligomeric assemblies using Robetta in CASP12. Proteins: Structure, Function and Bioinformatics, 2018, 86, 283-291.	2.6	49
63	Structure of the type VI secretion system TssKâ€“TssFâ€“TssG baseplate subcomplex revealed by cryo-electron microscopy. Nature Communications, 2018, 9, 5385.	12.8	37
64	Structural Insights into Mdn1, an Essential AAA Protein Required for Ribosome Biogenesis. Cell, 2018, 175, 822-834.e18.	28.9	42
65	Cryoâ€“electron microscopy structure of the lipid dropletâ€“formation protein seipin. Journal of Cell Biology, 2018, 217, 4080-4091.	5.2	147
66	Near-atomic model of microtubule-tau interactions. Science, 2018, 360, 1242-1246.	12.6	285
67	cryoem-cloud-tools: A software platform to deploy and manage cryo-EM jobs in the cloud. Journal of Structural Biology, 2018, 203, 230-235.	2.8	19
68	Germline VRC01 antibody recognition of a modified clade C HIV-1 envelope trimer and a glycosylated HIV-1 gp120 core. ELife, 2018, 7, .	6.0	32
69	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.	7.1	51
70	RosettaES: a sampling strategy enabling automated interpretation of difficult cryo-EM maps. Nature Methods, 2017, 14, 797-800.	19.0	118
71	The Therapeutic Antibody LM609 Selectively Inhibits Ligand Binding to Human Î±VÎ²3 Integrin via Steric Hindrance. Structure, 2017, 25, 1732-1739.e5.	3.3	24
72	Structural basis of TIR-domain-assembly formation in MAL- and MyD88-dependent TLR4 signaling. Nature Structural and Molecular Biology, 2017, 24, 743-751.	8.2	140

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73	Structural basis for the initiation of eukaryotic transcription-coupled DNA repair. Nature, 2017, 551, 653-657.	27.8	151
74	Cryo-EM structure of the protein-conducting ERAD channel Hrd1 in complex with Hrd3. Nature, 2017, 548, 352-355.	27.8	160
75	Modeling oblong proteins and waterâ€mediated interfaces with RosettaDock in CAPRI rounds 28â€“35. Proteins: Structure, Function and Bioinformatics, 2017, 85, 479-486.	2.6	18
76	Crucial steps in the structure determination of a coronavirus spike glycoprotein using cryoâ€electron microscopy. Protein Science, 2017, 26, 113-121.	7.6	31
77	Anti-diabetic drug binding site in a mammalian KATP channel revealed by Cryo-EM. ELife, 2017, 6, .	6.0	122
78	Rosetta Structure Prediction as a Tool for Solving Difficult Molecular Replacement Problems. Methods in Molecular Biology, 2017, 1607, 455-466.	0.9	11
79	Model for a novel membrane envelope in a filamentous hyperthermophilic virus. ELife, 2017, 6, .	6.0	37
80	Tools for Model Building and Optimization into Near-Atomic Resolution Electron Cryo-Microscopy Density Maps. Methods in Enzymology, 2016, 579, 255-276.	1.0	28
81	Improving hybrid statistical and physical forcefields through local structure enumeration. Protein Science, 2016, 25, 1525-1534.	7.6	6
82	<scp>CASP</scp>11 refinement experiments with <scp>ROSETTA</scp>. Proteins: Structure, Function and Bioinformatics, 2016, 84, 314-322.	2.6	26
83	Improved de novo structure prediction in <scp>CASP</scp>11 by incorporating coevolution information into Rosetta. Proteins: Structure, Function and Bioinformatics, 2016, 84, 67-75.	2.6	96
84	De novo design of protein homo-oligomers with modular hydrogen-bond networkâ€mediated specificity. Science, 2016, 352, 680-687.	12.6	262
85	Protocols for Molecular Modeling with Rosetta3 and RosettaScripts. Biochemistry, 2016, 55, 4748-4763.	2.5	182
86	Glycan shield and epitope masking of a coronavirus spike protein observed by cryo-electron microscopy. Nature Structural and Molecular Biology, 2016, 23, 899-905.	8.2	366
87	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.	9.7	128
88	Simultaneous Optimization of Biomolecular Energy Functions on Features from Small Molecules and Macromolecules. Journal of Chemical Theory and Computation, 2016, 12, 6201-6212.	5.3	382
89	Structure of a Chaperone-Usher Pilus Reveals the Molecular Basis of Rod Uncoiling. Cell, 2016, 164, 269-278.	28.9	61
90	Cryo-electron microscopy structure of a coronavirus spike glycoprotein trimer. Nature, 2016, 531, 114-117.	27.8	453

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91	Automated structure refinement of macromolecular assemblies from cryo-EM maps using Rosetta. ELife, 2016, 5, .	6.0	407
92	A virus that infects a hyperthermophile encapsidates A-form DNA. Science, 2015, 348, 914-917.	12.6	98
93	The Origin of Consistent Protein Structure Refinement from Structural Averaging. Structure, 2015, 23, 1123-1128.	3.3	16
94	Structure of EspB from the ESX-1 Type VII Secretion System and Insights into its Export Mechanism. Structure, 2015, 23, 571-583.	3.3	85
95	Combined Covalent-Electrostatic Model of Hydrogen Bonding Improves Structure Prediction with Rosetta. Journal of Chemical Theory and Computation, 2015, 11, 609-622.	5.3	204
96	Structure of the Type VI Secretion System Contractile Sheath. Cell, 2015, 160, 952-962.	28.9	216
97	De novo protein structure determination from near-atomic-resolution cryo-EM maps. Nature Methods, 2015, 12, 335-338.	19.0	172
98	Designing Two-Dimensional Protein Arrays through Fusion of Multimers and Interface Mutations. Nano Letters, 2015, 15, 5235-5239.	9.1	38
99	The molecular basis for flexibility in the flexible filamentous plant viruses. Nature Structural and Molecular Biology, 2015, 22, 642-644.	8.2	72
100	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.	7.1	72
101	Design of ordered two-dimensional arrays mediated by noncovalent protein-protein interfaces. Science, 2015, 348, 1365-1368.	12.6	219
102	Atomic-accuracy models from 4.5-Ã... cryo-electron microscopy data with density-guided iterative local refinement. Nature Methods, 2015, 12, 361-365.	19.0	313
103	EMRinger: side chainâ€“directed model and map validation for 3D cryo-electron microscopy. Nature Methods, 2015, 12, 943-946.	19.0	799
104	High thermodynamic stability of parametrically designed helical bundles. Science, 2014, 346, 481-485.	12.6	264
105	Crystal structure analysis of EstA from Arthrobacter sp. Rue61a â€“ an insight into catalytic promiscuity. FEBS Letters, 2014, 588, 1154-1160.	2.8	14
106	One contact for every twelve residues allows robust and accurate topologyâ€level protein structure modeling. Proteins: Structure, Function and Bioinformatics, 2014, 82, 208-218.	2.6	87
107	Relaxation of backbone bond geometry improves protein energy landscape modeling. Protein Science, 2014, 23, 47-55.	7.6	323
108	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.	2.8	30

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109	Improved low-resolution crystallographic refinement with Phenix and Rosetta. Nature Methods, 2013, 10, 1102-1104.	19.0	175
110	High-Resolution Comparative Modeling with RosettaCM. Structure, 2013, 21, 1735-1742.	3.3	1,010
111	Advances, Interactions, and Future Developments in the CNS, Phenix, and Rosetta Structural Biology Software Systems. Annual Review of Biophysics, 2013, 42, 265-287.	10.0	88
112	Cryoâ€EM model validation using independent map reconstructions. Protein Science, 2013, 22, 865-868.	7.6	72
113	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
114	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, 11648-11653.	7.1	59
115	A Refined Model of the Prototypical Salmonella SPI-1 T3SS Basal Body Reveals the Molecular Basis for Its Assembly. PLoS Pathogens, 2013, 9, e1003307.	4.7	76
116	Advances inRosettastructure prediction for difficult molecular-replacement problems. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 2202-2208.	2.5	20
117	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, 7899-7904.	7.1	51
118	The dynamic disulphide relay of quiescin sulphydryl oxidase. Nature, 2012, 488, 414-418.	27.8	70
119	phenix.mr_rosetta: molecular replacement and model rebuilding with Phenix and Rosetta. Journal of Structural and Functional Genomics, 2012, 13, 81-90.	1.2	131
120	Determination of the Structures of Symmetric Protein Oligomers from NMR Chemical Shifts and Residual Dipolar Couplings. Journal of the American Chemical Society, 2011, 133, 6288-6298.	13.7	65
121	Crystal structure of a monomeric retroviral protease solved by protein folding game players. Nature Structural and Molecular Biology, 2011, 18, 1175-1177.	8.2	463
122	Alternate States of Proteins Revealed by Detailed Energy Landscape Mapping. Journal of Molecular Biology, 2011, 405, 607-618.	4.2	324
123	Crystal structure of XMRV protease differs from the structures of other retropepsins. Nature Structural and Molecular Biology, 2011, 18, 227-229.	8.2	27
124	Improved molecular replacement by density- and energy-guided protein structure optimization. Nature, 2011, 473, 540-543.	27.8	226
125	Cryo-EM Structure of a Group II Chaperonin in the Prehydrolysis ATP-Bound State Leading to Lid Closure. Structure, 2011, 19, 633-639.	3.3	52
126	High-resolution structure of a retroviral protease folded as a monomer. Acta Crystallographica Section D: Biological Crystallography, 2011, 67, 907-914.	2.5	22

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127	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, 14879-14884.	7.1	123
128	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, 1355-1360.	7.1	191
129	Modeling Symmetric Macromolecular Structures in Rosetta3. PLoS ONE, 2011, 6, e20450.	2.5	197
130	Analyses of Subnanometer Resolution Cryo-EM Density Maps. Methods in Enzymology, 2010, 483, 1-29.	1.0	22
131	Refinement of Protein Structures into Low-Resolution Density Maps Using Rosetta. Journal of Molecular Biology, 2009, 392, 181-190.	4.2	272
132	Spherical-harmonic decomposition for molecular recognition in electron-density maps. International Journal of Data Mining and Bioinformatics, 2009, 3, 205.	0.1	6