

Matteo Dal Peraro

List of Publications by Year in descending order

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Version: 2024-02-01

112
papers

5,763
citations

76326

40
h-index

95266

68
g-index

127
all docs

127
docs citations

127
times ranked

8144
citing authors

#	ARTICLE	IF	CITATIONS
1	Biological nanopores for single-molecule sensing. <i>IScience</i> , 2022, 25, 104145.	4.1	25
2	Ultrasensitive Label-Free Detection of Protein-Membrane Interaction Exemplified by Toxin-Liposome Insertion. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3197-3201.	4.6	2
3	Online tools to easily build virtual molecular models for display in augmented and virtual reality on the web. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 114, 108164.	2.4	20
4	State-of-the-art web services for <i>de novo</i> protein structure prediction. <i>Briefings in Bioinformatics</i> , 2021, 22, .	6.5	13
5	CLoNe: automated clustering based on local density neighborhoods for application to biomolecular structural ensembles. <i>Bioinformatics</i> , 2021, 37, 921-928.	4.1	8
6	Assessment of transferable forcefields for protein simulations attests improved description of disordered states and secondary structure propensities, and hints at multi-protein systems as the next challenge for optimization. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 2626-2636.	4.1	25
7	Palmitoylated acyl protein thioesterase APT2 deforms membranes to extract substrate acyl chains. <i>Nature Chemical Biology</i> , 2021, 17, 438-447.	8.0	31
8	MolecularARweb: A Web Site for Chemistry and Structural Biology Education through Interactive Augmented Reality out of the Box in Commodity Devices. <i>Journal of Chemical Education</i> , 2021, 98, 2243-2255.	2.3	26
9	Investigating Crosstalk Among PTMs Provides Novel Insight Into the Structural Basis Underlying the Differential Effects of Nt17 PTMs on Mutant Httex1 Aggregation. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 686086.	3.5	8
10	Specific Protein-Membrane Interactions Promote Packaging of Metallo- β -Lactamases into Outer Membrane Vesicles. <i>Antimicrobial Agents and Chemotherapy</i> , 2021, 65, e0050721.	3.2	10
11	Extensive tissue-specific expression variation and novel regulators underlying circadian behavior. <i>Science Advances</i> , 2021, 7, .	10.3	21
12	Democratizing interactive, immersive experiences for science education with WebXR. <i>Nature Computational Science</i> , 2021, 1, 631-632.	8.0	13
13	S-acylation controls SARS-CoV-2 membrane lipid organization and enhances infectivity. <i>Developmental Cell</i> , 2021, 56, 2790-2807.e8.	7.0	80
14	<i>BET1</i> variants establish impaired vesicular transport as a cause for muscular dystrophy with epilepsy. <i>EMBO Molecular Medicine</i> , 2021, 13, e13787.	6.9	9
15	Prolyl endopeptidase-like is a (thio)esterase involved in mitochondrial respiratory chain function. <i>IScience</i> , 2021, 24, 103460.	4.1	8
16	Editorial: Multiscale Modeling From Macromolecules to Cell: Opportunities and Challenges of Biomolecular Simulations. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 194.	3.5	8
17	The Polyglutamine Expansion at the N-Terminal of Huntingtin Protein Modulates the Dynamic Configuration and Phosphorylation of the C-Terminal HEAT Domain. <i>Structure</i> , 2020, 28, 1035-1050.e8.	3.3	24
18	Ligand Binding to the Collagen VI Receptor Triggers a Talin-to-RhoA Switch that Regulates Receptor Endocytosis. <i>Developmental Cell</i> , 2020, 53, 418-430.e4.	7.0	12

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19	Molecular Bases of the Membrane Association Mechanism Potentiating Antibiotic Resistance by New Delhi Metallo- β -lactamase 1. <i>ACS Infectious Diseases</i> , 2020, 6, 2719-2731.	3.8	11
20	The Human RNA Helicase DDX21 Presents a Dimerization Interface Necessary for Helicase Activity. <i>IScience</i> , 2020, 23, 101811.	4.1	15
21	Aerolysin nanopores decode digital information stored in tailored macromolecular analytes. <i>Science Advances</i> , 2020, 6, .	10.3	57
22	Btk SH2-kinase interface is critical for allosteric kinase activation and its targeting inhibits B-cell neoplasms. <i>Nature Communications</i> , 2020, 11, 2319.	12.8	23
23	Will Cryo-Electron Microscopy Shift the Current Paradigm in Protein Structure Prediction?. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2443-2447.	5.4	8
24	Salt Enhances the Thermostability of Enteroviruses by Stabilizing Capsid Protein Interfaces. <i>Journal of Virology</i> , 2020, 94, .	3.4	15
25	Modelling structures in cryo-EM maps. <i>Current Opinion in Structural Biology</i> , 2019, 58, 105-114.	5.7	53
26	A further leap of improvement in tertiary structure prediction in CASP13 prompts new routes for future assessments. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 1100-1112.	2.6	73
27	Editorial overview: The future after the cryo-EM resolution revolution. <i>Current Opinion in Structural Biology</i> , 2019, 58, iii-iv.	5.7	1
28	Active Site-Induced Evolutionary Constraints Follow Fold Polarity Principles in Soluble Globular Enzymes. <i>Molecular Biology and Evolution</i> , 2019, 36, 1728-1733.	8.9	7
29	Transmembrane Prolines Mediate Signal Sensing and Decoding in <i>Bacillus subtilis</i> DesK Histidine Kinase. <i>MBio</i> , 2019, 10, .	4.1	21
30	Single-molecule sensing of peptides and nucleic acids by engineered aerolysin nanopores. <i>Nature Communications</i> , 2019, 10, 4918.	12.8	74
31	An Isoprene Lipid-Binding Protein Promotes Eukaryotic Coenzyme Q Biosynthesis. <i>Molecular Cell</i> , 2019, 73, 763-774.e10.	9.7	37
32	KAP1 is an antiparallel dimer with a functional asymmetry. <i>Life Science Alliance</i> , 2019, 2, e201900349.	2.8	16
33	Nucleo-cytosolic Shuttling of ARGONAUTE1 Prompts a Revised Model of the Plant MicroRNA Pathway. <i>Molecular Cell</i> , 2018, 69, 709-719.e5.	9.7	193
34	Assessment of data-assisted prediction by inclusion of crosslinking/mass spectrometry and small angle X-ray scattering data in the 12 th Critical Assessment of protein Structure Prediction experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 215-227.	2.6	4
35	Definition and classification of evaluation units for tertiary structure prediction in CASP12 facilitated through semi-automated metrics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 16-26.	2.6	12
36	Recruitment of the amyloid precursor protein by β -secretase at the synaptic plasma membrane. <i>Biochemical and Biophysical Research Communications</i> , 2018, 498, 334-341.	2.1	17

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37	Conserved Lipid and Small-Molecule Modulation of COQ8 Reveals Regulation of the Ancient Kinase-like UbiB Family. <i>Cell Chemical Biology</i> , 2018, 25, 154-165.e11.	5.2	63
38	Assessment of hard target modeling in CASP12 reveals an emerging role of alignment-based contact prediction methods. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 97-112.	2.6	79
39	Mapping the sensing spots of aerolysin for single oligonucleotides analysis. <i>Nature Communications</i> , 2018, 9, 2823.	12.8	60
40	COQ9 Membrane Association and Its Role in Coenzyme Q Biosynthesis. <i>FASEB Journal</i> , 2018, 32, 815.8.	0.5	0
41	Evolution of Acid-Sensing Olfactory Circuits in Drosophilids. <i>Neuron</i> , 2017, 93, 661-676.e6.	8.1	182
42	Signal Sensing and Transduction by Histidine Kinases as Unveiled through Studies on a Temperature Sensor. <i>Accounts of Chemical Research</i> , 2017, 50, 1359-1366.	15.6	46
43	Protein post-translational modifications: In silico prediction tools and molecular modeling. <i>Computational and Structural Biotechnology Journal</i> , 2017, 15, 307-319.	4.1	145
44	Structural, physicochemical and dynamic features conserved within the aerolysin pore-forming toxin family. <i>Scientific Reports</i> , 2017, 7, 13932.	3.3	38
45	Functional assays for the assessment of the pathogenicity of variants in GOSR2, an ER-to-Golgi SNARE involved in progressive myoclonus epilepsies. <i>DMM Disease Models and Mechanisms</i> , 2017, 10, 1391-1398.	2.4	11
46	Disentangling constraints using viability evolution principles in integrative modeling of macromolecular assemblies. <i>Scientific Reports</i> , 2017, 7, 235.	3.3	12
47	A Biologically-validated HCV E1E2 Heterodimer Structural Model. <i>Scientific Reports</i> , 2017, 7, 214.	3.3	32
48	Transcriptional regulatory logic of the diurnal cycle in the mouse liver. <i>PLoS Biology</i> , 2017, 15, e2001069.	5.6	68
49	Detection and sequence/structure mapping of biophysical constraints to protein variation in saturated mutational libraries and protein sequence alignments with a dedicated server. <i>BMC Bioinformatics</i> , 2016, 17, 242.	2.6	18
50	Immobilization of the N-terminal helix stabilizes prefusion paramyxovirus fusion proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E3844-51.	7.1	4
51	Cryo-EM structure of aerolysin variants reveals a novel protein fold and the pore-formation process. <i>Nature Communications</i> , 2016, 7, 12062.	12.8	144
52	Cooperative motion of a key positively charged residue and metal ions for DNA replication catalyzed by human DNA Polymerase- β . <i>Nucleic Acids Research</i> , 2016, 44, 2827-2836.	14.5	44
53	Effect of the Synaptic Plasma Membrane on the Stability of the Amyloid Precursor Protein Homodimer. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3572-3578.	4.6	16
54	Molecular Effects of Concentrated Solutes on Protein Hydration, Dynamics, and Electrostatics. <i>Biophysical Journal</i> , 2016, 111, 743-755.	0.5	29

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55	Cerebellar Ataxia and Coenzyme Q Deficiency through Loss of Unorthodox Kinase Activity. <i>Molecular Cell</i> , 2016, 63, 608-620.	9.7	101
56	A rheostat mechanism governs the bifurcation of carbon flux in mycobacteria. <i>Nature Communications</i> , 2016, 7, 12527.	12.8	27
57	Olfactory receptor pseudo-pseudogenes. <i>Nature</i> , 2016, 539, 93-97.	27.8	140
58	Pore-forming toxins: ancient, but never really out of fashion. <i>Nature Reviews Microbiology</i> , 2016, 14, 77-92.	28.6	600
59	A coiled coil switch mediates cold sensing by the thermosensory protein <i><scp>DesK</scp></i> . <i>Molecular Microbiology</i> , 2015, 98, 258-271.	2.5	50
60	How Structural and Physicochemical Determinants Shape Sequence Constraints in a Functional Enzyme. <i>PLoS ONE</i> , 2015, 10, e0118684.	2.5	41
61	Crystal structure of Hop2â€Mnd1 and mechanistic insights into its role in meiotic recombination. <i>Nucleic Acids Research</i> , 2015, 43, 3841-3856.	14.5	42
62	<i><i>LipidBuilder</i></i> : A Framework To Build Realistic Models for Biological Membranes. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2491-2499.	5.4	17
63	Catalytic Metal Ions and Enzymatic Processing of DNA and RNA. <i>Accounts of Chemical Research</i> , 2015, 48, 220-228.	15.6	130
64	Assessing the potential of atomistic molecular dynamics simulations to probe reversible protein-protein recognition and binding. <i>Scientific Reports</i> , 2015, 5, 10549.	3.3	50
65	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. <i>Structure</i> , 2015, 23, 1156-1167.	3.3	159
66	The importance of dynamics in integrative modeling of supramolecular assemblies. <i>Current Opinion in Structural Biology</i> , 2015, 31, 28-34.	5.7	20
67	GtrA Protein Rv3789 Is Required for Arabinosylation of Arabinogalactan in <i>Mycobacterium tuberculosis</i> . <i>Journal of Bacteriology</i> , 2015, 197, 3686-3697.	2.2	26
68	ComEA Is Essential for the Transfer of External DNA into the Periplasm in Naturally Transformable <i>Vibrio cholerae</i> Cells. <i>PLoS Genetics</i> , 2014, 10, e1004066.	3.5	107
69	New Strategies for Integrative Dynamic Modeling of Macromolecular Assembly. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014, 96, 77-111.	2.3	11
70	Critical roles of isoleucine-364 and adjacent residues in a hydrophobic gate control of phospholipid transport by the mammalian P4-ATPase ATP8A2. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, E1334-43.	7.1	103
71	Functional Dissection of Intersubunit Interactions in the EspR Virulence Regulator of <i>Mycobacterium tuberculosis</i> . <i>Journal of Bacteriology</i> , 2014, 196, 1889-1900.	2.2	9
72	Perturbations of the Straight Transmembrane α -Helical Structure of the Amyloid Precursor Protein Affect Its Processing by β -Secretase. <i>Journal of Biological Chemistry</i> , 2014, 289, 6763-6774.	3.4	39

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73	Molecular dynamics simulations of apocupredoxins: insights into the formation and stabilization of copper sites under entatic control. <i>Journal of Biological Inorganic Chemistry</i> , 2014, 19, 565-575.	2.6	19
74	HCV E2 core structures and mAbs: something is still missing. <i>Drug Discovery Today</i> , 2014, 19, 1964-1970.	6.4	27
75	Dissecting the Effects of Concentrated Carbohydrate Solutions on Protein Diffusion, Hydration, and Internal Dynamics. <i>Journal of Physical Chemistry B</i> , 2014, 118, 5310-5321.	2.6	24
76	A dimerization interface mediated by functionally critical residues creates interfacial disulfide bonds and copper sites in CueP. <i>Journal of Inorganic Biochemistry</i> , 2014, 140, 199-201.	3.5	5
77	Reaction Mechanism and Catalytic Fingerprint of Allantoin Racemase. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7457-7466.	2.6	5
78	Macromolecular Symmetric Assembly Prediction Using Swarm Intelligence Dynamic Modeling. <i>Structure</i> , 2013, 21, 1097-1106.	3.3	33
79	Molecular assembly of the aerolysin pore reveals a swirling membrane-insertion mechanism. <i>Nature Chemical Biology</i> , 2013, 9, 623-629.	8.0	183
80	Electrostatic-Consistent Coarse-Grained Potentials for Molecular Simulations of Proteins. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3515-3526.	5.3	29
81	In-Depth Analysis of Hyaline Fibromatosis Syndrome Frameshift Mutations at the Same Site Reveal the Necessity of Personalized Therapy. <i>Human Mutation</i> , 2013, 34, 1005-1017.	2.5	14
82	Cardiolipin Models for Molecular Simulations of Bacterial and Mitochondrial Membranes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 670-678.	5.3	30
83	Arranged Sevenfold: Structural Insights into the C-Terminal Oligomerization Domain of Human C4b-Binding Protein. <i>Journal of Molecular Biology</i> , 2013, 425, 1302-1317.	4.2	69
84	Molecular Simulations Highlight the Role of Metals in Catalysis and Inhibition of Type II Topoisomerase. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 857-862.	5.3	45
85	Assembly of the Transmembrane Domain of <i>E. coli</i> PhoQ Histidine Kinase: Implications for Signal Transduction from Molecular Simulations. <i>PLoS Computational Biology</i> , 2013, 9, e1002878.	3.2	42
86	TAL Effectors Specificity Stems from Negative Discrimination. <i>PLoS ONE</i> , 2013, 8, e80261.	2.5	17
87	In situ structural analysis of the <i>Yersinia enterocolitica</i> injectisome. <i>ELife</i> , 2013, 2, e00792.	6.0	109
88	The Lipopolysaccharide from <i>Campylobacter jejuni</i> Reveals an Unexpected Role of the Core-Oligosaccharide in MD-2 Binding. <i>PLoS Pathogens</i> , 2012, 8, e1002667.	4.7	32
89	Palmitoylated calnexin is a key component of the ribosome-translocon complex. <i>EMBO Journal</i> , 2012, 31, 1823-1835.	7.8	152
90	Atypical DNA recognition mechanism used by the EspR virulence regulator of <i>Mycobacterium tuberculosis</i> . <i>Molecular Microbiology</i> , 2011, 82, 251-264.	2.5	22

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91	Dual Chaperone Role of the C-Terminal Propeptide in Folding and Oligomerization of the Pore-Forming Toxin Aerolysin. <i>PLoS Pathogens</i> , 2011, 7, e1002135.	4.7	64
92	Length control of the injectisome needle requires only one molecule of Yop secretion protein P (YscP). <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 13860-13865.	7.1	43
93	Understanding the Effect of Magnesium Ion Concentration on the Catalytic Activity of Ribonuclease H through Computation: Does a Third Metal Binding Site Modulate Endonuclease Catalysis?. <i>Journal of the American Chemical Society</i> , 2010, 132, 13702-13712.	13.7	49
94	A Nonradial Coarse-Grained Potential for Proteins Produces Naturally Stable Secondary Structure Elements. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 315-324.	5.3	48
95	Challenges and Perspectives in Biomolecular Simulations: From the Atomistic Picture to Multiscale Modeling. <i>Chimia</i> , 2009, 63, 14.	0.6	15
96	Molecular dynamics calculations suggest a conduction mechanism for the M2 proton channel from influenza A virus. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 1069-1074.	7.1	111
97	The helical content of the YscP molecular ruler determines the length of the <i>Yersinia</i> injectisome. <i>Molecular Microbiology</i> , 2009, 71, 692-701.	2.5	34
98	Unraveling the Catalytic Pathway of Metalloenzyme Farnesyltransferase through QM/MM Computation. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1657-1666.	5.3	35
99	Common Mechanistic Features among Metallo- β -lactamases. <i>Journal of Biological Chemistry</i> , 2009, 284, 28164-28171.	3.4	54
100	Solution NMR Structure of a Designed Metalloprotein and Complementary Molecular Dynamics Refinement. <i>Structure</i> , 2008, 16, 210-215.	3.3	38
101	Phosphodiester Cleavage in Ribonuclease H Occurs via an Associative Two-Metal-Aided Catalytic Mechanism. <i>Journal of the American Chemical Society</i> , 2008, 130, 10955-10962.	13.7	134
102	Topologically Based Multipolar Reconstruction of Electrostatic Interactions in Multiscale Simulations of Proteins. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1378-1385.	5.3	28
103	The Metallo- β -lactamase GOB Is a Mono-Zn(II) Enzyme with a Novel Active Site. <i>Journal of Biological Chemistry</i> , 2007, 282, 18286-18293.	3.4	70
104	Proton Shuttles and Phosphatase Activity in Soluble Epoxide Hydrolase. <i>Journal of the American Chemical Society</i> , 2007, 129, 387-394.	13.7	60
105	Role of Zinc Content on the Catalytic Efficiency of B1 Metallo- β -Lactamases. <i>Journal of the American Chemical Society</i> , 2007, 129, 2808-2816.	13.7	80
106	Polarization effects and charge transfer in the KcsA potassium channel. <i>Biophysical Chemistry</i> , 2006, 124, 292-301.	2.8	84
107	Solute-Solvent Charge Transfer in Aqueous Solution. <i>ChemPhysChem</i> , 2005, 6, 1715-1718.	2.1	75
108	Substrate binding to mononuclear metallo- β -lactamase from <i>Bacillus cereus</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 54, 412-423.	2.6	39

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109	Water-Assisted Reaction Mechanism of Monozinc β -Lactamases. <i>Journal of the American Chemical Society</i> , 2004, 126, 12661-12668.	13.7	99
110	Protonation State of Asp120 in the Binuclear Active Site of the Metallo- β -Lactamase from <i>Bacteroides fragilis</i> . <i>Inorganic Chemistry</i> , 2003, 42, 4245-4247.	4.0	35
111	Structural determinants and hydrogen-bond network of the mononuclear zinc(II)- β -lactamase active site. <i>Journal of Biological Inorganic Chemistry</i> , 2002, 7, 704-712.	2.6	40
112	Ser133 phosphate-KIX interactions in the CREB-CBP complex: an ab initio molecular dynamics study. <i>European Biophysics Journal</i> , 2001, 30, 75-81.	2.2	13