

# Matteo Dal Peraro

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3819356/publications.pdf>

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	Pore-forming toxins: ancient, but never really out of fashion. <i>Nature Reviews Microbiology</i> , 2016, 14, 77-92.	28.6	600
2	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
3	Molecular assembly of the aerolysin pore reveals a swirling membrane-insertion mechanism. <i>Nature Chemical Biology</i> , 2013, 9, 623-629.	8.0	183
4	Evolution of Acid-Sensing Olfactory Circuits in Drosophilids. <i>Neuron</i> , 2017, 93, 661-676.e6.	8.1	182
5	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. <i>Structure</i> , 2015, 23, 1156-1167.	3.3	159
6	Palmitoylated calnexin is a key component of the ribosome-translocon complex. <i>EMBO Journal</i> , 2012, 31, 1823-1835.	7.8	152
7	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
8	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
9	Olfactory receptor pseudo-pseudogenes. <i>Nature</i> , 2016, 539, 93-97.	27.8	140
10	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
11	Catalytic Metal Ions and Enzymatic Processing of DNA and RNA. <i>Accounts of Chemical Research</i> , 2015, 48, 220-228.	15.6	130
12	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
13	In situ structural analysis of the <i>Yersinia enterocolitica</i> injectisome. <i>ELife</i> , 2013, 2, e00792.	6.0	109
14	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
15	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
16	Cerebellar Ataxia and Coenzyme Q Deficiency through Loss of Unorthodox Kinase Activity. <i>Molecular Cell</i> , 2016, 63, 608-620.	9.7	101
17	Water-Assisted Reaction Mechanism of Monozinc $\hat{\text{I}}^2$ -Lactamases. <i>Journal of the American Chemical Society</i> , 2004, 126, 12661-12668.	13.7	99
18	Polarization effects and charge transfer in the KcsA potassium channel. <i>Biophysical Chemistry</i> , 2006, 124, 292-301.	2.8	84

#	ARTICLE	IF	CITATIONS
19	Role of Zinc Content on the Catalytic Efficiency of B1 Metallo- $\beta$ -Lactamases. <i>Journal of the American Chemical Society</i> , 2007, 129, 2808-2816.	13.7	80
20	S-acylation controls SARS-CoV-2 membrane lipid organization and enhances infectivity. <i>Developmental Cell</i> , 2021, 56, 2790-2807.e8.	7.0	80
21	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
22	Solute-Solvent Charge Transfer in Aqueous Solution. <i>ChemPhysChem</i> , 2005, 6, 1715-1718.	2.1	75
23	Single-molecule sensing of peptides and nucleic acids by engineered aerolysin nanopores. <i>Nature Communications</i> , 2019, 10, 4918.	12.8	74
24	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
25	The Metallo- $\beta$ -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
26	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
27	Transcriptional regulatory logic of the diurnal cycle in the mouse liver. <i>PLoS Biology</i> , 2017, 15, e2001069.	5.6	68
28	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
29	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
30	Proton Shuttles and Phosphatase Activity in Soluble Epoxide Hydrolase. <i>Journal of the American Chemical Society</i> , 2007, 129, 387-394.	13.7	60
31	Mapping the sensing spots of aerolysin for single oligonucleotides analysis. <i>Nature Communications</i> , 2018, 9, 2823.	12.8	60
32	Aerolysin nanopores decode digital information stored in tailored macromolecular analytes. <i>Science Advances</i> , 2020, 6, .	10.3	57
33	Common Mechanistic Features among Metallo- $\beta$ -Lactamases. <i>Journal of Biological Chemistry</i> , 2009, 284, 28164-28171.	3.4	54
34	Modelling structures in cryo-EM maps. <i>Current Opinion in Structural Biology</i> , 2019, 58, 105-114.	5.7	53
35	A coiled coil switch mediates cold sensing by the thermosensory protein <i>&lt;scp&gt;DesK&lt;/scp&gt;</i> . <i>Molecular Microbiology</i> , 2015, 98, 258-271.	2.5	50
36	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

#	ARTICLE	IF	CITATIONS
37	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
38	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
39	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
40	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
41	Cooperative motion of a key positively charged residue and metal ions for DNA replication catalyzed by human DNA Polymerase- $\delta$ . <i>Nucleic Acids Research</i> , 2016, 44, 2827-2836.	14.5	44
42	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
43	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
44	Crystal structure of Hop2-Mnd1 and mechanistic insights into its role in meiotic recombination. <i>Nucleic Acids Research</i> , 2015, 43, 3841-3856.	14.5	42
45	How Structural and Physicochemical Determinants Shape Sequence Constraints in a Functional Enzyme. <i>PLoS ONE</i> , 2015, 10, e0118684.	2.5	41
46	Structural determinants and hydrogen-bond network of the mononuclear zinc(II)- $\beta$ -lactamase active site. <i>Journal of Biological Inorganic Chemistry</i> , 2002, 7, 704-712.	2.6	40
47	Substrate binding to mononuclear metallo- $\beta$ -lactamase from <i>Bacillus cereus</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 54, 412-423.	2.6	39
48	Perturbations of the Straight Transmembrane $\alpha$ -Helical Structure of the Amyloid Precursor Protein Affect Its Processing by $\beta$ -Secretase. <i>Journal of Biological Chemistry</i> , 2014, 289, 6763-6774.	3.4	39
49	Solution NMR Structure of a Designed Metalloprotein and Complementary Molecular Dynamics Refinement. <i>Structure</i> , 2008, 16, 210-215.	3.3	38
50	Structural, physicochemical and dynamic features conserved within the aerolysin pore-forming toxin family. <i>Scientific Reports</i> , 2017, 7, 13932.	3.3	38
51	An Isoprene Lipid-Binding Protein Promotes Eukaryotic Coenzyme Q Biosynthesis. <i>Molecular Cell</i> , 2019, 73, 763-774.e10.	9.7	37
52	Protonation State of Asp120 in the Binuclear Active Site of the Metallo- $\beta$ -Lactamase from <i>Bacteroides fragilis</i> . <i>Inorganic Chemistry</i> , 2003, 42, 4245-4247.	4.0	35
53	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
54	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

#	ARTICLE	IF	CITATIONS
55	Macromolecular Symmetric Assembly Prediction Using Swarm Intelligence Dynamic Modeling. <i>Structure</i> , 2013, 21, 1097-1106.	3.3	33
56	The Lipopolysaccharide from <i>Capnocytophaga canimorsus</i> Reveals an Unexpected Role of the Core-Oligosaccharide in MD-2 Binding. <i>PLoS Pathogens</i> , 2012, 8, e1002667.	4.7	32
57	A Biologically-validated HCV E1E2 Heterodimer Structural Model. <i>Scientific Reports</i> , 2017, 7, 214.	3.3	32
58	Palmitoylated acyl protein thioesterase APT2 deforms membranes to extract substrate acyl chains. <i>Nature Chemical Biology</i> , 2021, 17, 438-447.	8.0	31
59	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
60	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
61	Molecular Effects of Concentrated Solutes on Protein Hydration, Dynamics, and Electrostatics. <i>Biophysical Journal</i> , 2016, 111, 743-755.	0.5	29
62	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
63	HCV E2 core structures and mAbs: something is still missing. <i>Drug Discovery Today</i> , 2014, 19, 1964-1970.	6.4	27
64	A rheostat mechanism governs the bifurcation of carbon flux in mycobacteria. <i>Nature Communications</i> , 2016, 7, 12527.	12.8	27
65	CtrA 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
66	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
67	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
68	Biological nanopores for single-molecule sensing. <i>IScience</i> , 2022, 25, 104145.	4.1	25
69	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
70	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
71	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
72	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

#	ARTICLE	IF	CITATIONS
73	Transmembrane Prolines Mediate Signal Sensing and Decoding in Bacillus subtilis DesK Histidine Kinase. MBio, 2019, 10, .	4.1	21
74	Extensive tissue-specific expression variation and novel regulators underlying circadian behavior. Science Advances, 2021, 7, .	10.3	21
75	The importance of dynamics in integrative modeling of supramolecular assemblies. Current Opinion in Structural Biology, 2015, 31, 28-34.	5.7	20
76	Online tools to easily build virtual molecular models for display in augmented and virtual reality on the web. Journal of Molecular Graphics and Modelling, 2022, 114, 108164.	2.4	20
77	Molecular dynamics simulations of apocupredoxins: insights into the formation and stabilization of copper sites under entatic control. Journal of Biological Inorganic Chemistry, 2014, 19, 565-575.	2.6	19
78	Detection and sequence/structure mapping of biophysical constraints to protein variation in saturated mutational libraries and protein sequence alignments with a dedicated server. BMC Bioinformatics, 2016, 17, 242.	2.6	18
79	TAL Effectors Specificity Stems from Negative Discrimination. PLoS ONE, 2013, 8, e80261.	2.5	17
80	<i>LipidBuilder</i>: A Framework To Build Realistic Models for Biological Membranes. Journal of Chemical Information and Modeling, 2015, 55, 2491-2499.	5.4	17
81	Recruitment of the amyloid precursor protein by $\beta$ -secretase at the synaptic plasma membrane. Biochemical and Biophysical Research Communications, 2018, 498, 334-341.	2.1	17
82	Effect of the Synaptic Plasma Membrane on the Stability of the Amyloid Precursor Protein Homodimer. Journal of Physical Chemistry Letters, 2016, 7, 3572-3578.	4.6	16
83	KAP1 is an antiparallel dimer with a functional asymmetry. Life Science Alliance, 2019, 2, e201900349.	2.8	16
84	Challenges and Perspectives in Biomolecular Simulations: From the Atomistic Picture to Multiscale Modeling. Chimia, 2009, 63, 14.	0.6	15
85	The Human RNA Helicase DDX21 Presents a Dimerization Interface Necessary for Helicase Activity. IScience, 2020, 23, 101811.	4.1	15
86	Salt Enhances the Thermostability of Enteroviruses by Stabilizing Capsid Protein Interfaces. Journal of Virology, 2020, 94, .	3.4	15
87	In-Depth Analysis of Hyaline Fibromatosis Syndrome Frameshift Mutations at the Same Site Reveal the Necessity of Personalized Therapy. Human Mutation, 2013, 34, 1005-1017.	2.5	14
88	Ser133 phosphate-KIX interactions in the CREB-CBP complex: an ab initio molecular dynamics study. European Biophysics Journal, 2001, 30, 75-81.	2.2	13
89	State-of-the-art web services for <i>de novo</i> protein structure prediction. Briefings in Bioinformatics, 2021, 22, .	6.5	13
90	Democratizing interactive, immersive experiences for science education with WebXR. Nature Computational Science, 2021, 1, 631-632.	8.0	13

#	ARTICLE	IF	CITATIONS
91	Disentangling constraints using viability evolution principles in integrative modeling of macromolecular assemblies. <i>Scientific Reports</i> , 2017, 7, 235.	3.3	12
92	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
93	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
94	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
95	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
96	Molecular Bases of the Membrane Association Mechanism Potentiating Antibiotic Resistance by New Delhi Metallo- $\beta$ -lactamase 1. <i>ACS Infectious Diseases</i> , 2020, 6, 2719-2731.	3.8	11
97	Specific Protein-Membrane Interactions Promote Packaging of Metallo- $\beta$ -Lactamases into Outer Membrane Vesicles. <i>Antimicrobial Agents and Chemotherapy</i> , 2021, 65, e0050721.	3.2	10
98	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
99	<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
100	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
101	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
102	CLoNe: automated clustering based on local density neighborhoods for application to biomolecular structural ensembles. <i>Bioinformatics</i> , 2021, 37, 921-928.	4.1	8
103	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
104	Prolyl endopeptidase-like is a (thio)esterase involved in mitochondrial respiratory chain function. <i>IScience</i> , 2021, 24, 103460.	4.1	8
105	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
106	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
107	Reaction Mechanism and Catalytic Fingerprint of Allantoin Racemase. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7457-7466.	2.6	5
108	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

#	ARTICLE	IF	CITATIONS
109	Assessment of data-assisted prediction by inclusion of crosslinking/mass spectrometry and small angle X-ray scattering data in the 12 <sup>th</sup> Critical Assessment of protein Structure Prediction experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 215-227.	2.6	4
110	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
111	Editorial overview: The future after the cryo-EM resolution revolution. <i>Current Opinion in Structural Biology</i> , 2019, 58, iii-iv.	5.7	1
112	COQ9 Membrane Association and Its Role in Coenzyme Q Biosynthesis. <i>FASEB Journal</i> , 2018, 32, 815.8.	0.5	0