

# Matteo Dal Peraro

## List of Publications by Year in Descending Order

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**Version:** 2024-04-28

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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.

113  
papers

4,086  
citations

36  
h-index

60  
g-index

127  
ext. papers

5,103  
ext. citations

8.4  
avg, IF

5.88  
L-index

#	Paper	IF	Citations
113	Biological nanopores for single-molecule sensing.. <i>IScience</i> , <b>2022</b> , 25, 104145	6.1	1
112	Ultrasensitive Label-Free Detection of Protein-Membrane Interaction Exemplified by Toxin-Liposome Insertion.. <i>Journal of Physical Chemistry Letters</i> , <b>2022</b> , 3197-3201	6.4	1
111	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> , <b>2022</b> , 114, 108164	2.8	1
110	BET1 variants establish impaired vesicular transport as a cause for muscular dystrophy with epilepsy. <i>EMBO Molecular Medicine</i> , <b>2021</b> , 13, e13787	12	1
109	Prolyl endopeptidase-like is a (thio)esterase involved in mitochondrial respiratory chain function. <i>IScience</i> , <b>2021</b> , 24, 103460	6.1	0
108	Democratizing interactive, immersive experiences for science education with WebXR. <i>Nature Computational Science</i> , <b>2021</b> , 1, 631-632		1
107	S-acylation controls SARS-CoV-2 membrane lipid organization and enhances infectivity. <i>Developmental Cell</i> , <b>2021</b> , 56, 2790-2807.e8	10.2	10
106	Molecularweb: 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> , <b>2021</b> , 98, 2243-2255	2.4	5
105	Investigating Crosstalk Among PTMs Provides Novel Insight Into the Structural Basis Underlying the Differential Effects of Nε17 PTMs on Mutant Httex1 Aggregation. <i>Frontiers in Molecular Biosciences</i> , <b>2021</b> , 8, 686086	5.6	3
104	State-of-the-art web services for de novo protein structure prediction. <i>Briefings in Bioinformatics</i> , <b>2021</b> , 22,	13.4	5
103	CLoNe: automated clustering based on local density neighborhoods for application to biomolecular structural ensembles. <i>Bioinformatics</i> , <b>2021</b> , 37, 921-928	7.2	2
102	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> , <b>2021</b> , 19, 2626-2636	6.8	9
101	Palmitoylated acyl protein thioesterase APT2 deforms membranes to extract substrate acyl chains. <i>Nature Chemical Biology</i> , <b>2021</b> , 17, 438-447	11.7	9
100	Specific Protein-Membrane Interactions Promote Packaging of Metallo-β-Lactamases into Outer Membrane Vesicles. <i>Antimicrobial Agents and Chemotherapy</i> , <b>2021</b> , 65, e0050721	5.9	2
99	Extensive tissue-specific expression variation and novel regulators underlying circadian behavior. <i>Science Advances</i> , <b>2021</b> , 7,	14.3	7
98	The Human RNA Helicase DDX21 Presents a Dimerization Interface Necessary for Helicase Activity. <i>IScience</i> , <b>2020</b> , 23, 101811	6.1	6
97	Aerolysin nanopores decode digital information stored in tailored macromolecular analytes. <i>Science Advances</i> , <b>2020</b> , 6,	14.3	16

96	Btk SH2-kinase interface is critical for allosteric kinase activation and its targeting inhibits B-cell neoplasms. <i>Nature Communications</i> , <b>2020</b> , 11, 2319	17.4	12
95	Will Cryo-Electron Microscopy Shift the Current Paradigm in Protein Structure Prediction?. <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 2443-2447	6.1	5
94	Salt Enhances the Thermostability of Enteroviruses by Stabilizing Capsid Protein Interfaces. <i>Journal of Virology</i> , <b>2020</b> , 94,	6.6	4
93	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> , <b>2020</b> , 28, 1035-1050.e8	5.2	7
92	Ligand Binding to the Collagen VI Receptor Triggers a Talin-to-RhoA Switch that Regulates Receptor Endocytosis. <i>Developmental Cell</i> , <b>2020</b> , 53, 418-430.e4	10.2	5
91	Molecular Bases of the Membrane Association Mechanism Potentiating Antibiotic Resistance by New Delhi Metallo-βactamase 1. <i>ACS Infectious Diseases</i> , <b>2020</b> , 6, 2719-2731	5.5	7
90	Active Site-Induced Evolutionary Constraints Follow Fold Polarity Principles in Soluble Globular Enzymes. <i>Molecular Biology and Evolution</i> , <b>2019</b> , 36, 1728-1733	8.3	5
89	Modelling structures in cryo-EM maps. <i>Current Opinion in Structural Biology</i> , <b>2019</b> , 58, 105-114	8.1	24
88	A further leap of improvement in tertiary structure prediction in CASP13 prompts new routes for future assessments. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2019</b> , 87, 1100-1112	4.2	50
87	KAP1 is an antiparallel dimer with a functional asymmetry. <i>Life Science Alliance</i> , <b>2019</b> , 2,	5.8	9
86	Transmembrane Prolines Mediate Signal Sensing and Decoding in Bacillus subtilis DesK Histidine Kinase. <i>MBio</i> , <b>2019</b> , 10,	7.8	7
85	Single-molecule sensing of peptides and nucleic acids by engineered aerolysin nanopores. <i>Nature Communications</i> , <b>2019</b> , 10, 4918	17.4	30
84	An Isoprene Lipid-Binding Protein Promotes Eukaryotic Coenzyme Q Biosynthesis. <i>Molecular Cell</i> , <b>2019</b> , 73, 763-774.e10	17.6	20
83	Nucleo-cytosolic Shuttling of ARGONAUTE1 Prompts a Revised Model of the Plant MicroRNA Pathway. <i>Molecular Cell</i> , <b>2018</b> , 69, 709-719.e5	17.6	118
82	Assessment of data-assisted prediction by inclusion of crosslinking/mass-spectrometry and small angle X-ray scattering data in the 12 Critical Assessment of protein Structure Prediction experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2018</b> , 86 Suppl 1, 215-227	4.2	2
81	Definition and classification of evaluation units for tertiary structure prediction in CASP12 facilitated through semi-automated metrics. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2018</b> , 86 Suppl 1, 16-26	4.2	10
80	Mapping the sensing spots of aerolysin for single oligonucleotides analysis. <i>Nature Communications</i> , <b>2018</b> , 9, 2823	17.4	47
79	COQ9 Membrane Association and Its Role in Coenzyme Q Biosynthesis. <i>FASEB Journal</i> , <b>2018</b> , 32, 815.8	0.9	

78	Recruitment of the amyloid precursor protein by $\beta$ -secretase at the synaptic plasma membrane. <i>Biochemical and Biophysical Research Communications</i> , <b>2018</b> , 498, 334-341	3.4	10
77	Conserved Lipid and Small-Molecule Modulation of COQ8 Reveals Regulation of the Ancient Kinase-like UbiB Family. <i>Cell Chemical Biology</i> , <b>2018</b> , 25, 154-165.e11	8.2	40
76	Assessment of hard target modeling in CASP12 reveals an emerging role of alignment-based contact prediction methods. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2018</b> , 86 Suppl 1, 97-112	4.2	57
75	Evolution of Acid-Sensing Olfactory Circuits in Drosophilids. <i>Neuron</i> , <b>2017</b> , 93, 661-676.e6	13.9	103
74	Signal Sensing and Transduction by Histidine Kinases as Unveiled through Studies on a Temperature Sensor. <i>Accounts of Chemical Research</i> , <b>2017</b> , 50, 1359-1366	24.3	31
73	Protein post-translational modifications: prediction tools and molecular modeling. <i>Computational and Structural Biotechnology Journal</i> , <b>2017</b> , 15, 307-319	6.8	96
72	Structural, physicochemical and dynamic features conserved within the aerolysin pore-forming toxin family. <i>Scientific Reports</i> , <b>2017</b> , 7, 13932	4.9	21
71	Functional assays for the assessment of the pathogenicity of variants of GOSR2, an ER-to-Golgi SNARE involved in progressive myoclonus epilepsies. <i>DMM Disease Models and Mechanisms</i> , <b>2017</b> , 10, 1391-1398	4.1	9
70	Transcriptional regulatory logic of the diurnal cycle in the mouse liver. <i>PLoS Biology</i> , <b>2017</b> , 15, e2001069	9.7	51
69	Disentangling constraints using viability evolution principles in integrative modeling of macromolecular assemblies. <i>Scientific Reports</i> , <b>2017</b> , 7, 235	4.9	10
68	A Biologically-validated HCV E1E2 Heterodimer Structural Model. <i>Scientific Reports</i> , <b>2017</b> , 7, 214	4.9	21
67	Effect of the Synaptic Plasma Membrane on the Stability of the Amyloid Precursor Protein Homodimer. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 3572-8	6.4	13
66	Molecular Effects of Concentrated Solutes on Protein Hydration, Dynamics, and Electrostatics. <i>Biophysical Journal</i> , <b>2016</b> , 111, 743-755	2.9	24
65	Cerebellar Ataxia and Coenzyme Q Deficiency through Loss of Unorthodox Kinase Activity. <i>Molecular Cell</i> , <b>2016</b> , 63, 608-620	17.6	67
64	A rheostat mechanism governs the bifurcation of carbon flux in mycobacteria. <i>Nature Communications</i> , <b>2016</b> , 7, 12527	17.4	21
63	Olfactory receptor pseudo-pseudogenes. <i>Nature</i> , <b>2016</b> , 539, 93-97	50.4	71
62	Pore-forming toxins: ancient, but never really out of fashion. <i>Nature Reviews Microbiology</i> , <b>2016</b> , 14, 77-92	22.2	407
61	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> , <b>2016</b> , 17, 242	3.6	11

60	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> , <b>2016</b> , 113, E3844-51	11.5	4
59	Cryo-EM structure of aerolysin variants reveals a novel protein fold and the pore-formation process. <i>Nature Communications</i> , <b>2016</b> , 7, 12062	17.4	108
58	Cooperative motion of a key positively charged residue and metal ions for DNA replication catalyzed by human DNA Polymerase- $\beta$ . <i>Nucleic Acids Research</i> , <b>2016</b> , 44, 2827-36	20.1	28
57	Assessing the potential of atomistic molecular dynamics simulations to probe reversible protein-protein recognition and binding. <i>Scientific Reports</i> , <b>2015</b> , 5, 10549	4.9	39
56	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. <i>Structure</i> , <b>2015</b> , 23, 1156-67	5.2	131
55	The importance of dynamics in integrative modeling of supramolecular assemblies. <i>Current Opinion in Structural Biology</i> , <b>2015</b> , 31, 28-34	8.1	17
54	GtrA Protein Rv3789 Is Required for Arabinosylation of Arabinogalactan in Mycobacterium tuberculosis. <i>Journal of Bacteriology</i> , <b>2015</b> , 197, 3686-97	3.5	19
53	A coiled coil switch mediates cold sensing by the thermosensory protein DesK. <i>Molecular Microbiology</i> , <b>2015</b> , 98, 258-71	4.1	43
52	How structural and physicochemical determinants shape sequence constraints in a functional enzyme. <i>PLoS ONE</i> , <b>2015</b> , 10, e0118684	3.7	28
51	Crystal structure of Hop2-Mnd1 and mechanistic insights into its role in meiotic recombination. <i>Nucleic Acids Research</i> , <b>2015</b> , 43, 3841-56	20.1	27
50	LipidBuilder: A Framework To Build Realistic Models for Biological Membranes. <i>Journal of Chemical Information and Modeling</i> , <b>2015</b> , 55, 2491-9	6.1	13
49	Catalytic metal ions and enzymatic processing of DNA and RNA. <i>Accounts of Chemical Research</i> , <b>2015</b> , 48, 220-8	24.3	106
48	Molecular dynamics simulations of apocupredoxins: insights into the formation and stabilization of copper sites under entatic control. <i>Journal of Biological Inorganic Chemistry</i> , <b>2014</b> , 19, 565-75	3.7	14
47	HCV E2 core structures and mAbs: something is still missing. <i>Drug Discovery Today</i> , <b>2014</b> , 19, 1964-70	8.8	24
46	Dissecting the effects of concentrated carbohydrate solutions on protein diffusion, hydration, and internal dynamics. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 5310-21	3.4	21
45	A dimerization interface mediated by functionally critical residues creates interfacial disulfide bonds and copper sites in CueP. <i>Journal of Inorganic Biochemistry</i> , <b>2014</b> , 140, 199-201	4.2	5
44	Reaction Mechanism and Catalytic Fingerprint of Allantoin Racemase. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 7457-7466	3.4	4
43	ComEA is essential for the transfer of external DNA into the periplasm in naturally transformable <i>Vibrio cholerae</i> cells. <i>PLoS Genetics</i> , <b>2014</b> , 10, e1004066	6	76

42	New strategies for integrative dynamic modeling of macromolecular assembly. <i>Advances in Protein Chemistry and Structural Biology</i> , <b>2014</b> , 96, 77-111	5.3	8
41	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> , <b>2014</b> , 111, E1334-43	11.5	76
40	Functional dissection of intersubunit interactions in the EspR virulence regulator of Mycobacterium tuberculosis. <i>Journal of Bacteriology</i> , <b>2014</b> , 196, 1889-900	3.5	6
39	Perturbations of the straight transmembrane helical structure of the amyloid precursor protein affect its processing by $\beta$ secretase. <i>Journal of Biological Chemistry</i> , <b>2014</b> , 289, 6763-6774	5.4	30
38	Macromolecular symmetric assembly prediction using swarm intelligence dynamic modeling. <i>Structure</i> , <b>2013</b> , 21, 1097-1106	5.2	27
37	Molecular assembly of the aerolysin pore reveals a swirling membrane-insertion mechanism. <i>Nature Chemical Biology</i> , <b>2013</b> , 9, 623-9	11.7	150
36	Electrostatic-Consistent Coarse-Grained Potentials for Molecular Simulations of Proteins. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 3515-26	6.4	27
35	In-depth analysis of hyaline fibromatosis syndrome frameshift mutations at the same site reveal the necessity of personalized therapy. <i>Human Mutation</i> , <b>2013</b> , 34, 1005-17	4.7	13
34	Cardiolipin Models for Molecular Simulations of Bacterial and Mitochondrial Membranes. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 670-8	6.4	21
33	Arranged sevenfold: structural insights into the C-terminal oligomerization domain of human C4b-binding protein. <i>Journal of Molecular Biology</i> , <b>2013</b> , 425, 1302-17	6.5	54
32	Molecular Simulations Highlight the Role of Metals in Catalysis and Inhibition of Type II Topoisomerase. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 857-62	6.4	39
31	Assembly of the transmembrane domain of E. coli PhoQ histidine kinase: implications for signal transduction from molecular simulations. <i>PLoS Computational Biology</i> , <b>2013</b> , 9, e1002878	5	34
30	TAL effectors specificity stems from negative discrimination. <i>PLoS ONE</i> , <b>2013</b> , 8, e80261	3.7	14
29	In situ structural analysis of the Yersinia enterocolitica injectisome. <i>ELife</i> , <b>2013</b> , 2, e00792	8.9	86
28	The lipopolysaccharide from Capnocytophaga canimorsus reveals an unexpected role of the core-oligosaccharide in MD-2 binding. <i>PLoS Pathogens</i> , <b>2012</b> , 8, e1002667	7.6	28
27	Palmitoylated calnexin is a key component of the ribosome-translocon complex. <i>EMBO Journal</i> , <b>2012</b> , 31, 1823-35	13	116
26	Atypical DNA recognition mechanism used by the EspR virulence regulator of Mycobacterium tuberculosis. <i>Molecular Microbiology</i> , <b>2011</b> , 82, 251-64	4.1	20
25	Dual chaperone role of the C-terminal propeptide in folding and oligomerization of the pore-forming toxin aerolysin. <i>PLoS Pathogens</i> , <b>2011</b> , 7, e1002135	7.6	45

24	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> , <b>2010</b> , 107, 13860-5	11.5	30
23	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> , <b>2010</b> , 132, 13702-12	16.4	46
22	A Nonradial Coarse-Grained Potential for Proteins Produces Naturally Stable Secondary Structure Elements. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 315-24	6.4	42
21	Catalytic Mechanism of Metallo-β-Lactamases: Insights from Calculations and Experiments <b>2010</b> , 605-622		1
20	Challenges and Perspectives in Biomolecular Simulations: From the Atomistic Picture to Multiscale Modeling. <i>Chimia</i> , <b>2009</b> , 63, 14-18	1.3	11
19	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> , <b>2009</b> , 106, 1069-74	11.5	103
18	The helical content of the YscP molecular ruler determines the length of the Yersinia injectisome. <i>Molecular Microbiology</i> , <b>2009</b> , 71, 692-701	4.1	32
17	Unraveling the Catalytic Pathway of Metalloenzyme Farnesyltransferase through QM/MM Computation. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 1657-66	6.4	30
16	Common mechanistic features among metallo-beta-lactamases: a computational study of Aeromonas hydrophila CphA enzyme. <i>Journal of Biological Chemistry</i> , <b>2009</b> , 284, 28164-28171	5.4	50
15	Solution NMR structure of a designed metalloprotein and complementary molecular dynamics refinement. <i>Structure</i> , <b>2008</b> , 16, 210-5	5.2	32
14	Phosphodiester cleavage in ribonuclease H occurs via an associative two-metal-aided catalytic mechanism. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 10955-62	16.4	119
13	Topologically Based Multipolar Reconstruction of Electrostatic Interactions in Multiscale Simulations of Proteins. <i>Journal of Chemical Theory and Computation</i> , <b>2008</b> , 4, 1378-85	6.4	24
12	Role of zinc content on the catalytic efficiency of B1 metallo beta-lactamases. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 2808-16	16.4	77
11	The metallo-beta-lactamase GOB is a mono-Zn(II) enzyme with a novel active site. <i>Journal of Biological Chemistry</i> , <b>2007</b> , 282, 18286-18293	5.4	63
10	Proton shuttles and phosphatase activity in soluble epoxide hydrolase. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 387-94	16.4	52
9	Polarization effects and charge transfer in the KcsA potassium channel. <i>Biophysical Chemistry</i> , <b>2006</b> , 124, 292-301	3.5	78
8	Solute-solvent charge transfer in aqueous solution. <i>ChemPhysChem</i> , <b>2005</b> , 6, 1715-8	3.2	71
7	Substrate binding to mononuclear metallo-beta-lactamase from Bacillus cereus. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2004</b> , 54, 412-23	4.2	36

6	Water-assisted reaction mechanism of monozinc beta-lactamases. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 12661-8	16.4	92
5	Protonation state of Asp120 in the binuclear active site of the metallo-beta-lactamase from <i>Bacteroides fragilis</i> . <i>Inorganic Chemistry</i> , <b>2003</b> , 42, 4245-7	5.1	34
4	Structural determinants and hydrogen-bond network of the mononuclear zinc(II)-beta-lactamase active site. <i>Journal of Biological Inorganic Chemistry</i> , <b>2002</b> , 7, 704-12	3.7	39
3	Ser133 phosphate-KIX interactions in the CREB-CBP complex: an ab initio molecular dynamics study. <i>European Biophysics Journal</i> , <b>2001</b> , 30, 75-81	1.9	11
2	KAP1 is an antiparallel dimer with a natively functional asymmetry		2
1	S-acylation controls SARS-Cov-2 membrane lipid organization and enhances infectivity		3