Carlo Camilloni

List of Publications by Citations

109 papers	6,378 citations	37 h-index	79 g-index
134 ext. papers	8,075 ext. citations	6.3 avg, IF	6.44 L-index

#	Paper	IF	Citations
109	PLUMED 2: New feathers for an old bird. *Computer Physics Communications*, **2014**, 185, 604-613	4.2	1470
108	PLUMED: A portable plugin for free-energy calculations with molecular dynamics. *Computer Physics Communications*, **2009**, 180, 1961-1972	4.2	1087
107	Promoting transparency and reproducibility in enhanced molecular simulations. *Nature Methods*, **2019**, 16, 670-673	21.6	271
106	Determination of secondary structure populations in disordered states of proteins using nuclear magnetic resonance chemical shifts. *Biochemistry*, **2012**, 51, 2224-31	3.2	258
105	Principles of protein structural ensemble determination. *Current Opinion in Structural Biology*, **2017**, 42, 106-116	8.1	196
104	MobiDB 3.0: more annotations for intrinsic disorder, conformational diversity and interactions in proteins. *Nucleic Acids Research*, **2018**, 46, D471-D476	20.1	143
103	Molecular dynamics simulations with replica-averaged structural restraints generate structural ensembles according to the maximum entropy principle. *Journal of Chemical Physics*, **2013**, 138, 094112	3.9	143
102	Urea and guanidinium chloride denature protein L in different ways in molecular dynamics simulations. *Biophysical Journal*, **2008**, 94, 4654-61	2.9	129
101	Characterization of the free-energy landscapes of proteins by NMR-guided metadynamics. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 6817-22	11.5	112
100	Metainference: A Bayesian inference method for heterogeneous systems. *Science Advances*, **2016**, 2, e1501177	14.3	110
99	Dynamic binding mode of a Synaptotagmin-1-SNARE complex in solution. *Nature Structural and Molecular Biology*, **2015**, 22, 555-64	17.6	99
98	A structural ensemble of a ribosome-nascent chain complex during cotranslational protein folding. *Nature Structural and Molecular Biology*, **2016**, 23, 278-285	17.6	96
97	The inverted free energy landscape of an intrinsically disordered peptide by simulations and experiments. *Scientific Reports*, **2015**, 5, 15449	4.9	84
96	Simultaneous quantification of protein order and disorder. *Nature Chemical Biology*, **2017**, 13, 339-342	11.7	83
95	Molecular Recognition by Templated Folding of an Intrinsically Disordered Protein. *Scientific Reports*, **2016**, 6, 21994	4.9	77
94	Characterization of the conformational equilibrium between the two major substates of RNase A using NMR chemical shifts. *Journal of the American Chemical Society*, **2012**, 134, 3968-71	16.4	75
93	In-cell NMR characterization of the secondary structure populations of a disordered conformation of □synuclein within E. coli cells. *PLoS ONE*, **2013**, 8, e72286	3.7	70

92	Cryo-EM structure of cardiac amyloid fibrils from an immunoglobulin light chain AL amyloidosis patient. *Nature Communications*, **2019**, 10, 1269	17.4	68
91	Towards a structural biology of the hydrophobic effect in protein folding. *Scientific Reports*, **2016**, 6, 28285	4.9	62
90	The s2D method: simultaneous sequence-based prediction of the statistical populations of ordered and disordered regions in proteins. *Journal of Molecular Biology*, **2015**, 427, 982-996	6.5	60
89	Replica-Averaged Metadynamics. *Journal of Chemical Theory and Computation*, **2013**, 9, 5610-7	6.4	57
88	Exploring the protein G helix free-energy surface by solute tempering metadynamics. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 1647-54	4.2	56
87	Statistical mechanics of the denatured state of a protein using replica-averaged metadynamics. *Journal of the American Chemical Society*, **2014**, 136, 8982-91	16.4	53
86	Metadynamic metainference: Enhanced sampling of the metainference ensemble using metadynamics. *Scientific Reports*, **2016**, 6, 31232	4.9	52
85	Comparison of successive transition states for folding reveals alternative early folding pathways of two homologous proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 19241-6	11.5	52
84	The H50Q mutation induces a 10-fold decrease in the solubility of □synuclein. *Journal of Biological Chemistry*, **2015**, 290, 2395-404	5.4	51
83	Cyclophilin A catalyzes proline isomerization by an electrostatic handle mechanism. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 10203-8	11.5	49
82	Stabilization and structural analysis of a membrane-associated hIAPP aggregation intermediate. *ELife*, **2017**, 6,	8.9	47
81	Structure of a low-population binding intermediate in protein-RNA recognition. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 7171-6	11.5	46
80	Networks of Dynamic Allostery Regulate Enzyme Function. *Structure*, **2017**, 25, 276-286	5.2	45
79	A tensor-free method for the structural and dynamical refinement of proteins using residual dipolar couplings. *Journal of Physical Chemistry B*, **2015**, 119, 653-61	3.4	43
78	Integrative structural and dynamical biology with PLUMED-ISDB. *Bioinformatics*, **2017**, 33, 3999-4000	7.2	41
77	Rational design of mutations that change the aggregation rate of a protein while maintaining its native structure and stability. *Scientific Reports*, **2016**, 6, 25559	4.9	41
76	Structural basis for terminal loop recognition and stimulation of pri-miRNA-18a processing by hnRNP A1. *Nature Communications*, **2018**, 9, 2479	17.4	41
75	Conformational recognition of an intrinsically disordered protein. *Biophysical Journal*, **2014**, 106, 1771-9	2.9	40

74	Structural characterization of the interaction of □synuclein nascent chains with the ribosomal surface and trigger factor. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 5012-7	11.5	40
73	Sequence Specificity in the Entropy-Driven Binding of a Small Molecule and a Disordered Peptide. *Journal of Molecular Biology*, **2017**, 429, 2772-2779	6.5	38
72	Understanding the frustration arising from the competition between function, misfolding, and aggregation in a globular protein. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 14141-6	11.5	36
71	Assessment of the use of NMR chemical shifts as replica-averaged structural restraints in molecular dynamics simulations to characterize the dynamics of proteins. *Journal of Physical Chemistry B*, **2013**, 117, 1838-43	3.4	36
70	Metadynamic metainference: Convergence towards force field independent structural ensembles of a disordered peptide. *Journal of Chemical Physics*, **2017**, 146, 165102	3.9	35
69	Conformational dynamics in crystals reveal the molecular bases for D76N beta-2 microglobulin aggregation propensity. *Nature Communications*, **2018**, 9, 1658	17.4	35
68	Energy landscape of the prion protein helix 1 probed by metadynamics and NMR. *Biophysical Journal*, **2012**, 102, 158-67	2.9	34
67	Hierarchy of folding and unfolding events of protein G, CI2, and ACBP from explicit-solvent simulations. *Journal of Chemical Physics*, **2011**, 134, 045105	3.9	34
66	A structurally heterogeneous transition state underlies coupled binding and folding of disordered proteins. *Journal of Biological Chemistry*, **2019**, 294, 1230-1239	5.4	29
65	Small-molecule sequestration of amyloid-□as a drug discovery strategy for Alzheimer's disease. *Science Advances*, **2020**, 6,	14.3	28
64	Emergence and evolution of an interaction between intrinsically disordered proteins. *ELife*, **2017**, 6,	8.9	28
63	ALMOST: an all atom molecular simulation toolkit for protein structure determination. *Journal of Computational Chemistry*, **2014**, 35, 1101-5	3.5	28
62	Systematic mapping of free energy landscapes of a growing filamin domain during biosynthesis. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 9744-9749	11.5	26
61	A highly compliant protein native state with a spontaneous-like mechanical unfolding pathway. *Journal of the American Chemical Society*, **2012**, 134, 17068-75	16.4	24
60	Determination of the individual roles of the linker residues in the interdomain motions of calmodulin using NMR chemical shifts. *Journal of Molecular Biology*, **2014**, 426, 1826-38	6.5	21
59	Determination of Protein Structural Ensembles by Hybrid-Resolution SAXS Restrained Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2020**, 16, 2825-2834	6.4	20
58	Advanced simulation techniques for the thermodynamic and kinetic characterization of biological systems. *Advances in Physics: X*, **2018**, 3, 1477531	5.1	20
57	A conformational ensemble derived using NMR methyl chemical shifts reveals a mechanical clamping transition that gates the binding of the HU protein to DNA. *Journal of the American Chemical Society*, **2014**, 136, 2204-7	16.4	17

56	The dynamics of linear polyubiquitin. *Science Advances*, **2020**, 6,	14.3	17
55	Using Pseudocontact Shifts and Residual Dipolar Couplings as Exact NMR Restraints for the Determination of Protein Structural Ensembles. *Biochemistry*, **2015**, 54, 7470-6	3.2	16
54	The dynamics of interleukin-8 and its interaction with human CXC receptor I peptide. *Protein Science*, **2014**, 23, 464-80	6.3	16
53	Lymphotactin: how a protein can adopt two folds. *Journal of Chemical Physics*, **2009**, 131, 245105	3.9	16
52	Molecular dynamics ensemble refinement of the heterogeneous native state of NCBD using chemical shifts and NOEs. *PeerJ*, **2018**, 6, e5125	3.1	16
51	Structural Characterization of the Early Events in the Nucleation-Condensation Mechanism in a Protein Folding Process. *Journal of the American Chemical Society*, **2017**, 139, 6899-6910	16.4	15
50	Structure and dynamics of the integrin LFA-1 I-domain in the inactive state underlie its inside-out/outside-in signaling and allosteric mechanisms. *Structure*, **2015**, 23, 745-53	5.2	15
49	Identification and Structural Characterization of an Intermediate in the Folding of the Measles Virus X Domain. *Journal of Biological Chemistry*, **2016**, 291, 10886-92	5.4	15
48	The Antibody Light-Chain Linker Regulates Domain Orientation and Amyloidogenicity. *Journal of Molecular Biology*, **2018**, 430, 4925-4940	6.5	15
47	Mapping the Protein Fold Universe Using the CamTube Force Field in Molecular Dynamics Simulations. *PLoS Computational Biology*, **2015**, 11, e1004435	5	14
46	Early events in protein folding: Is there something more than hydrophobic burst?. *Protein Science*, **2008**, 17, 1424-33	6.3	14
45	Martini bead form factors for nucleic acids and their application in the refinement of protein□nucleic acid complexes against SAXS data. *Journal of Applied Crystallography*, **2019**, 52, 394-402	3.8	14
44	Refinement of □-Synuclein Ensembles Against SAXS Data: Comparison of Force Fields and Methods. *Frontiers in Molecular Biosciences*, **2021**, 8, 654333	5.6	14
43	The co-existence of cold activity and thermal stability in an Antarctic GH42 □-galactosidase relies on its hexameric quaternary arrangement. *FEBS Journal*, **2021**, 288, 546-565	5.7	14
42	Simultaneous NMR characterisation of multiple minima in the free energy landscape of an RNA UUCG tetraloop. *Physical Chemistry Chemical Physics*, **2017**, 19, 2797-2804	3.6	13
41	Structure and Dynamics of GeoCyp: A Thermophilic Cyclophilin with a Novel Substrate Binding Mechanism That Functions Efficiently at Low Temperatures. *Biochemistry*, **2015**, 54, 3207-17	3.2	13
40	A relationship between the aggregation rates of □-synuclein variants and the □-sheet populations in their monomeric forms. *Journal of Physical Chemistry B*, **2013**, 117, 10737-41	3.4	13
39	The PHR Family: The Role of Extracellular Transglycosylases in Shaping Candida albicans Cells. *Journal of Fungi (Basel, Switzerland)*, **2017**, 3,	5.6	13

38	A kinetic ensemble of the Alzheimer's Aβ peptide. *Nature Computational Science*, **2021**, 1, 71-78		13
37	Ratcheted molecular-dynamics simulations identify efficiently the transition state of protein folding. *Journal of Chemical Physics*, **2012**, 137, 235101	3.9	12
36	Archaeal MBF1 binds to 30S and 70S ribosomes via its helix-turn-helix domain. *Biochemical Journal*, **2014**, 462, 373-84	3.8	10
35	An implementation of the maximum-caliber principle by replica-averaged time-resolved restrained simulations. *Journal of Chemical Physics*, **2018**, 148, 184114	3.9	10
34	Atomistic simulations of the HIV-1 protease folding inhibition. *Biophysical Journal*, **2008**, 95, 550-62	2.9	9
33	From A to B: a ride in the free energy surfaces of protein G domains suggests how new folds arise. *Journal of Chemical Physics*, **2012**, 136, 185101	3.9	8
32	Structural Insight into IAPP-Derived Amyloid Inhibitors and Their Mechanism of Action. *Angewandte Chemie - International Edition*, **2020**, 59, 5771-5781	16.4	8
31	Determination of the conformational states of strychnine in solution using NMR residual dipolar couplings in a tensor-free approach. *Methods*, **2018**, 148, 4-8	4.6	7
30	NMR characterization of the conformational fluctuations of the human lymphocyte function-associated antigen-1 I-domain. *Protein Science*, **2014**, 23, 1596-606	6.3	7
29	Mapping the transition state for a binding reaction between ancient intrinsically disordered proteins. *Journal of Biological Chemistry*, **2020**, 295, 17698-17712	5.4	7
28	Structural Insights into the Calcium-Mediated Allosteric Transition in the C-Terminal Domain of Calmodulin from Nuclear Magnetic Resonance Measurements. *Biochemistry*, **2016**, 55, 19-28	3.2	6
27	Folding Mechanism of the SH3 Domain from Grb2. *Journal of Physical Chemistry B*, **2018**, 122, 11166-11173	3.4	6
26	New opportunities for tensor-free calculations of residual dipolar couplings for the study of protein dynamics. *Journal of Biomolecular NMR*, **2014**, 58, 233-8	3	6
25	Biochemical and biophysical comparison of human and mouse beta-2 microglobulin reveals the molecular determinants of low amyloid propensity. *FEBS Journal*, **2020**, 287, 546-560	5.7	6
24	A superposition free method for protein conformational ensemble analyses and local clustering based on a differential geometry representation of backbone. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 302-312	4.2	5
23	Reply to "Comment on "A Tensor-Free Method for the Structural and Dynamic Refinement of Proteins using Residual Dipolar Couplings"". *Journal of Physical Chemistry B*, **2015**, 119, 8225-8226	3.4	5
22	Sampling the Denatured State of Polypeptides in Water, Urea, and Guanidine Chloride to Strict Equilibrium Conditions with the Help of Massively Parallel Computers. *Journal of Chemical Theory and Computation*, **2014**, 10, 846-54	6.4	5
21	Optical absorption of a green fluorescent protein variant: environment effects in a density functional study. *Journal of Physical Chemistry B*, **2007**, 111, 10807-12	3.4	5

20	Small molecule sequestration of amyloid-β as a drug discovery strategy for Alzheimer's disease		4
19	MD Simulations of Intrinsically Disordered Proteins with Replica-Averaged Chemical Shift Restraints. *Biophysical Journal*, **2014**, 106, 481a	2.9	3
18	Metadynamic sampling of the free-energy landscapes of proteins coupled with a Monte Carlo algorithm. *Gene*, **2008**, 422, 37-40	3.8	3
17	A Practical Guide to the Simultaneous Determination of Protein Structure and Dynamics Using Metainference. *Methods in Molecular Biology*, **2019**, 2022, 313-340	1.4	3
16	Cryo-EM Structures of Azospirillum brasilense Glutamate Synthase in Its Oligomeric Assemblies. *Journal of Molecular Biology*, **2019**, 431, 4523-4526	6.5	2
15	Structural Basis of Inhibition of the Pioneer Transcription Factor NF-Y by Suramin. *Cells*, **2020**, 9,	7.9	2
14	Identification of the folding inhibitors of hen-egg lysozyme: gathering the right tools. *European Biophysics Journal*, **2010**, 39, 911-9	1.9	2
13	A kinetic ensemble of the Alzheimer's Aβ peptide		2
12	Converging experimental and computational views of the knotting mechanism of a small knotted protein. *Biophysical Journal*, **2021**, 120, 2276-2286	2.9	2
11	Properties of low-dimensional collective variables in the molecular dynamics of biopolymers. *Physical Review E*, **2016**, 94, 052406	2.4	2
10	A method for partitioning the information contained in a protein sequence between its structure and function. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86, 956-964	4.2	2
9	Structural Insight into IAPP-Derived Amyloid Inhibitors and Their Mechanism of Action. *Angewandte Chemie*, **2020**, 132, 5820-5830	3.6	1
8	Structural basis for terminal loop recognition and processing of pri-miRNA-18a by hnRNP A1		1
7	Conformational Stability and Dynamics in Crystals Recapitulate Protein Behavior in Solution. *Biophysical Journal*, **2020**, 119, 978-988	2.9	1
6	How to Determine Accurate Conformational Ensembles by Metadynamics Metainference: A Chignolin Study Case. *Frontiers in Molecular Biosciences*, **2021**, 8, 694130	5.6	1
5	Refinement of α-synuclein ensembles against SAXS data: Comparison of force fields and methods		1
4	High Conformational Flexibility of the E2F1/DP1/DNA Complex. *Journal of Molecular Biology*, **2021**, 433, 167119	6.5	1
3	Disordered Regions Flanking the Binding Interface Modulate Affinity between CBP and NCOA. *Journal of Molecular Biology*, **2022**, 434, 167643	6.5	1

2	Structural investigation of the folding of an immunoglobulin domain on the ribosome using NMR Spectroscopy (LB197). *FASEB Journal*, **2014**, 28, LB197	0.9
1	l- to d-Amino Acid Substitution in the Immunodominant LCMV-Derived Epitope gp33 Highlights the Sensitivity of the TCR Recognition Mechanism for the MHC/Peptide Structure and Dynamics.. *ACS Omega*, **2022**, 7, 9622-9635	3.9