Carlo Camilloni

List of Publications by Year
in descending order

115 papers	9,469 citations	76326 40 h-index	45317 90 g-index
134 all docs	134 docs citations	134 times ranked	9631 citing authors

#	Article	IF	Citations
1	PLUMED 2: New feathers for an old bird. Computer Physics Communications, 2014, 185, 604-613.	7.5	2,454
2	PLUMED: A portable plugin for free-energy calculations with molecular dynamics. Computer Physics Communications, 2009, 180, 1961-1972.	7.5	1,448
3	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
4	Determination of Secondary Structure Populations in Disordered States of Proteins Using Nuclear Magnetic Resonance Chemical Shifts. Biochemistry, 2012, 51, 2224-2231.	2.5	316
5	Principles of protein structural ensemble determination. Current Opinion in Structural Biology, 2017, 42, 106-116.	5.7	285
6	MobiDB 3.0: more annotations for intrinsic disorder, conformational diversity and interactions in proteins. Nucleic Acids Research, 2018, 46, D471-D476.	14.5	190
7	Metainference: A Bayesian inference method for heterogeneous systems. Science Advances, 2016, 2, e1501177.	10.3	180
8	Molecular dynamics simulations with replica-averaged structural restraints generate structural ensembles according to the maximum entropy principle. Journal of Chemical Physics, 2013, 138, 094112.	3.0	169
9	Urea and Guanidinium Chloride Denature Protein L in Different Ways in Molecular Dynamics Simulations. Biophysical Journal, 2008, 94, 4654-4661.	0.5	141
10	A structural ensemble of a ribosomeâ€“nascent chain complex during cotranslational protein folding. Nature Structural and Molecular Biology, 2016, 23, 278-285.	8.2	135
11	Dynamic binding mode of a Synaptotagmin-1â€“SNARE complex in solution. Nature Structural and Molecular Biology, 2015, 22, 555-564.	8.2	129
12	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, 6817-6822.	7.1	122
13	The inverted free energy landscape of an intrinsically disordered peptide by simulations and experiments. Scientific Reports, 2015, 5, 15449.	3.3	118
14	Simultaneous quantification of protein order and disorder. Nature Chemical Biology, 2017, 13, 339-342.	8.0	113
15	Cryo-EM structure of cardiac amyloid fibrils from an immunoglobulin light chain AL amyloidosis patient. Nature Communications, 2019, 10, 1269.	12.8	113
16	Small-molecule sequestration of amyloid-Î² as a drug discovery strategy for Alzheimerâ€™s disease. Science Advances, 2020, 6, .	10.3	95
17	Towards a structural biology of the hydrophobic effect in protein folding. Scientific Reports, 2016, 6, 28285.	3.3	91
18	In-Cell NMR Characterization of the Secondary Structure Populations of a Disordered Conformation of Î±-Synuclein within E. coli Cells. PLoS ONE, 2013, 8, e72286.	2.5	89

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19	Molecular Recognition by Templated Folding of an Intrinsically Disordered Protein. Scientific Reports, 2016, 6, 21994.	3.3	87
20	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, 3968-3971.	13.7	84
21	Structural basis for terminal loop recognition and stimulation of pri-miRNA-18a processing by hnRNP A1. Nature Communications, 2018, 9, 2479.	12.8	80
22	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.	4.2	77
23	Metadynamic metainference: Enhanced sampling of the metainference ensemble using metadynamics. Scientific Reports, 2016, 6, 31232.	3.3	76
24	Statistical Mechanics of the Denatured State of a Protein Using Replica-Averaged Metadynamics. Journal of the American Chemical Society, 2014, 136, 8982-8991.	13.7	69
25	Exploring the protein G helix freeâ€energy surface by solute tempering metadynamics. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1647-1654.	2.6	68
26	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, 10203-10208.	7.1	68
27	The H50Q Mutation Induces a 10-fold Decrease in the Solubility of Î±-Synuclein. Journal of Biological Chemistry, 2015, 290, 2395-2404.	3.4	65
28	Replica-Averaged Metadynamics. Journal of Chemical Theory and Computation, 2013, 9, 5610-5617.	5.3	64
29	Networks of Dynamic Allostery Regulate Enzyme Function. Structure, 2017, 25, 276-286.	3.3	63
30	Sequence Specificity in the Entropy-Driven Binding of a Small Molecule and a Disordered Peptide. Journal of Molecular Biology, 2017, 429, 2772-2779.	4.2	62
31	Stabilization and structural analysis of a membrane-associated hIAPP aggregation intermediate. ELife, 2017, 6, .	6.0	61
32	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, 19241-19246.	7.1	59
33	Integrative structural and dynamical biology with PLUMED-ISDB. Bioinformatics, 2017, 33, 3999-4000.	4.1	59
34	Structural characterization of the interaction of Î±-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, 5012-5017.	7.1	54
35	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, 7171-7176.	7.1	54
36	Conformational dynamics in crystals reveal the molecular bases for D76N beta-2 microglobulin aggregation propensity. Nature Communications, 2018, 9, 1658.	12.8	53

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37	A Tensor-Free Method for the Structural and Dynamical Refinement of Proteins using Residual Dipolar Couplings. Journal of Physical Chemistry B, 2015, 119, 653-661.	2.6	51
38	Refinement of Î±-Synuclein Ensembles Against SAXS Data: Comparison of Force Fields and Methods. Frontiers in Molecular Biosciences, 2021, 8, 654333.	3.5	51
39	Conformational Recognition of an Intrinsically Disordered Protein. Biophysical Journal, 2014, 106, 1771-1779.	0.5	47
40	Rational design of mutations that change the aggregation rate of a protein while maintaining its native structure and stability. Scientific Reports, 2016, 6, 25559.	3.3	47
41	Metadynamic metainference: Convergence towards force field independent structural ensembles of a disordered peptide. Journal of Chemical Physics, 2017, 146, 165102.	3.0	47
42	Hierarchy of folding and unfolding events of protein G, CI2, and ACBP from explicit-solvent simulations. Journal of Chemical Physics, 2011, 134, 045105.	3.0	45
43	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, 14141-14146.	7.1	43
44	Emergence and evolution of an interaction between intrinsically disordered proteins. ELife, 2017, 6, .	6.0	42
45	A kinetic ensemble of the Alzheimerâ€™s AÎ² peptide. Nature Computational Science, 2021, 1, 71-78.	8.0	42
46	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, 1838-1843.	2.6	41
47	Energy Landscape of the Prion Protein Helix 1 Probed by Metadynamics and NMR. Biophysical Journal, 2012, 102, 158-167.	0.5	39
48	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.	7.1	39
49	A structurally heterogeneous transition state underlies coupled binding and folding of disordered proteins. Journal of Biological Chemistry, 2019, 294, 1230-1239.	3.4	39
50	The dynamics of linear polyubiquitin. Science Advances, 2020, 6, .	10.3	38
51	Determination of Protein Structural Ensembles by Hybrid-Resolution SAXS Restrained Molecular Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 2825-2834.	5.3	33
52	ALMOST: An all atom molecular simulation toolkit for protein structure determination. Journal of Computational Chemistry, 2014, 35, 1101-1105.	3.3	31
53	The coâ€existence of cold activity and thermal stability in an Antarctic GH42 Î²â€galactosidase relies on its hexameric quaternary arrangement. FEBS Journal, 2021, 288, 546-565.	4.7	31
54	A Highly Compliant Protein Native State with a Spontaneous-like Mechanical Unfolding Pathway. Journal of the American Chemical Society, 2012, 134, 17068-17075.	13.7	29

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55	Advanced simulation techniques for the thermodynamic and kinetic characterization of biological systems. Advances in Physics: X, 2018, 3, 1477531.	4.1	29
56	The Antibody Light-Chain Linker Regulates Domain Orientation and Amyloidogenicity. Journal of Molecular Biology, 2018, 430, 4925-4940.	4.2	27
57	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, 1826-1838.	4.2	25
58	Molecular dynamics ensemble refinement of the heterogeneous native state of NCBD using chemical shifts and NOEs. PeerJ, 2018, 6, e5125.	2.0	25
59	A Small Molecule Stabilizes the Disordered Native State of the Alzheimerâ€™s AÎ² Peptide. ACS Chemical Neuroscience, 2022, 13, 1738-1745.	3.5	25
60	Ratcheted molecular-dynamics simulations identify efficiently the transition state of protein folding. Journal of Chemical Physics, 2012, 137, 235101.	3.0	24
61	Lymphotactin: How a protein can adopt two folds. Journal of Chemical Physics, 2009, 131, 245105.	3.0	22
62	The dynamics of interleukinâ€8 and its interaction with human CXC receptor I peptide. Protein Science, 2014, 23, 464-480.	7.6	21
63	The PHR Family: The Role of Extracellular Transglycosylases in Shaping Candida albicans Cells. Journal of Fungi (Basel, Switzerland), 2017, 3, 59.	3.5	21
64	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, 2204-2207.	13.7	20
65	Disordered Regions Flanking the Binding Interface Modulate Affinity between CBP and NCOA. Journal of Molecular Biology, 2022, 434, 167643.	4.2	20
66	Using Pseudocontact Shifts and Residual Dipolar Couplings as Exact NMR Restraints for the Determination of Protein Structural Ensembles. Biochemistry, 2015, 54, 7470-7476.	2.5	19
67	Martini bead form factors for nucleic acids and their application in the refinement of proteinâ€“nucleic acid complexes against SAXS data. Journal of Applied Crystallography, 2019, 52, 394-402.	4.5	19
68	Structure and Dynamics of GeoCyp: A Thermophilic Cyclophilin with a Novel Substrate Binding Mechanism That Functions Efficiently at Low Temperatures. Biochemistry, 2015, 54, 3207-3217.	2.5	18
69	Identification and Structural Characterization of an Intermediate in the Folding of the Measles Virus X Domain. Journal of Biological Chemistry, 2016, 291, 10886-10892.	3.4	18
70	Structural Characterization of the Early Events in the Nucleationâ€“Condensation Mechanism in a Protein Folding Process. Journal of the American Chemical Society, 2017, 139, 6899-6910.	13.7	18
71	Simultaneous NMR characterisation of multiple minima in the free energy landscape of an RNA UUCG tetraloop. Physical Chemistry Chemical Physics, 2017, 19, 2797-2804.	2.8	18
72	Mapping the Protein Fold Universe Using the CamTube Force Field in Molecular Dynamics Simulations. PLoS Computational Biology, 2015, 11, e1004435.	3.2	17

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73	Structural Insight into IAPPâ€Derived Amyloid Inhibitors and Their Mechanism of Action. Angewandte Chemie - International Edition, 2020, 59, 5771-5781.	13.8	17
74	Archaeal MBF1 binds to 30S and 70S ribosomes via its helixâ€“turnâ€“helix domain. Biochemical Journal, 2014, 462, 373-384.	3.7	16
75	An implementation of the maximum-caliber principle by replica-averaged time-resolved restrained simulations. Journal of Chemical Physics, 2018, 148, 184114.	3.0	16
76	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, 745-753.	3.3	15
77	Early events in protein folding: Is there something more than hydrophobic burst?. Protein Science, 2008, 17, 1424-1433.	7.6	14
78	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.	3.0	14
79	A Relationship between the Aggregation Rates of Î±-Synuclein Variants and the Î²-Sheet Populations in Their Monomeric Forms. Journal of Physical Chemistry B, 2013, 117, 10737-10741.	2.6	13
80	Determination of the conformational states of strychnine in solution using NMR residual dipolar couplings in a tensor-free approach. Methods, 2018, 148, 4-8.	3.8	13
81	Atomistic Simulations of the HIV-1 Protease Folding Inhibition. Biophysical Journal, 2008, 95, 550-562.	0.5	12
82	Converging experimental and computational views of the knotting mechanism of a small knotted protein. Biophysical Journal, 2021, 120, 2276-2286.	0.5	12
83	Mapping the transition state for a binding reaction between ancient intrinsically disordered proteins. Journal of Biological Chemistry, 2020, 295, 17698-17712.	3.4	12
84	Biochemical and biophysical comparison of human and mouse betaâ€2 microglobulin reveals the molecular determinants of low amyloid propensity. FEBS Journal, 2020, 287, 546-560.	4.7	11
85	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.	2.5	9
86	Folding Mechanism of the SH3 Domain from Grb2. Journal of Physical Chemistry B, 2018, 122, 11166-11173.	2.6	9
87	New opportunities for tensor-free calculations of residual dipolar couplings for the study of protein dynamics. Journal of Biomolecular NMR, 2014, 58, 233-238.	2.8	8
88	NMR characterization of the conformational fluctuations of the human lymphocyte functionâ€associated antigenâ€1 Iâ€domain. Protein Science, 2014, 23, 1596-1606.	7.6	8
89	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.	2.6	8
90	Structural Basis of Inhibition of the Pioneer Transcription Factor NF-Y by Suramin. Cells, 2020, 9, 2370.	4.1	8

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91	Multi- e GO: An in silico lens to look into protein aggregation kinetics at atomic resolution. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	7
92	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, 846-854.	5.3	6
93	Reply to â€œComment on â€˜A Tensor-Free Method for the Structural and Dynamic Refinement of Proteins using Residual Dipolar Couplingsâ€™â€. Journal of Physical Chemistry B, 2015, 119, 8225-8226.	2.6	6
94	Inactivation of the Pyrimidine Biosynthesis pyrD Gene Negatively Affects Biofilm Formation and Virulence Determinants in the Crohnâ€™s Disease-Associated Adherent Invasive Escherichia coli LF82 Strain. Microorganisms, 2022, 10, 537.	3.6	6
95	Optical Absorption of a Green Fluorescent Protein Variant:â€‰ Environment Effects in a Density Functional Study. Journal of Physical Chemistry B, 2007, 111, 10807-10812.	2.6	5
96	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.	2.6	5
97	How to Determine Accurate Conformational Ensembles by Metadynamics Metainference: A Chignolin Study Case. Frontiers in Molecular Biosciences, 2021, 8, 694130.	3.5	5
98	Properties of low-dimensional collective variables in the molecular dynamics of biopolymers. Physical Review E, 2016, 94, 052406.	2.1	4
99	Cryo-EM Structures of AzospirillumÂbrasilense Glutamate Synthase in Its Oligomeric Assemblies. Journal of Molecular Biology, 2019, 431, 4523-4526.	4.2	4
100	High Conformational Flexibility of the E2F1/DP1/DNA Complex. Journal of Molecular Biology, 2021, 433, 167119.	4.2	4
101	Metadynamic sampling of the free-energy landscapes of proteins coupled with a Monte Carlo algorithm. Gene, 2008, 422, 37-40.	2.2	3
102	MD Simulations of Intrinsically Disordered Proteins with Replica-Averaged Chemical Shift Restraints. Biophysical Journal, 2014, 106, 481a.	0.5	3
103	Conformational Stability and Dynamics in Crystals Recapitulate Protein Behavior in Solution. Biophysical Journal, 2020, 119, 978-988.	0.5	3
104	Structural Insight into IAPPâ€Derived Amyloid Inhibitors and Their Mechanism of Action. Angewandte Chemie, 2020, 132, 5820-5830.	2.0	3
105	A Practical Guide to the Simultaneous Determination of Protein Structure and Dynamics Using Metainference. Methods in Molecular Biology, 2019, 2022, 313-340.	0.9	3
106	Identification of the folding inhibitors of hen-egg lysozyme: gathering the right tools. European Biophysics Journal, 2010, 39, 911-919.	2.2	2
107	Thermodynamics of an Intrinsically Disordered Protein by Atomistic Simulations. Biophysical Journal, 2013, 104, 55a.	0.5	1
108	Characterization of Protein Kinase a Free Energy Landscape by NMR-Restrained Metadynamics. Biophysical Journal, 2017, 112, 50a.	0.5	1

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109	<scp>l</scp>- to <scp>d</scp>-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.	3.5	1
110	Determination of the Individual Roles of the Linker Residues in the Inter-Domain Motions of Calmodulin using NMR Chemical Shifts. Biophysical Journal, 2014, 106, 636a.	0.5	0
111	Conformational Equilibrium between the Sub States of the Acidic Denatured State of ACBP Determined by NMR Chemical Shifts and Metadynamics. Biophysical Journal, 2014, 106, 459a-460a.	0.5	0
112	Structural Investigation of an Immunoglobulin Domain on the Ribosome using NMR Spectroscopy. Biophysical Journal, 2017, 112, 41a.	0.5	0
113	Probing Specificity in Disordered Protein Interactions with Small Molecules using Integrative Methods. Biophysical Journal, 2019, 116, 180a.	0.5	0
114	Integrative Methods for Protein Dynamics and Aggregation. Biophysical Journal, 2019, 116, 50a.	0.5	0
115	Structural investigation of the folding of an immunoglobulin domain on the ribosome using NMR Spectroscopy (LB197). FASEB Journal, 2014, 28, LB197.	0.5	0