Carlo Camilloni

List of Publications by Year
in descending order

115 papers	9,469 citations	76196 40 h-index	45213 90 g-index
134 all docs	134 docs citations	134 times ranked	9631 citing authors

#	Article	IF	Citations
1	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.	1.6	6
2	<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.	1.6	1
3	A Small Molecule Stabilizes the Disordered Native State of the Alzheimerâ€™s AÎ² Peptide. ACS Chemical Neuroscience, 2022, 13, 1738-1745.	1.7	25
4	Disordered Regions Flanking the Binding Interface Modulate Affinity between CBP and NCOA. Journal of Molecular Biology, 2022, 434, 167643.	2.0	20
5	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, .	3.3	7
6	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.	2.2	31
7	A kinetic ensemble of the Alzheimerâ€™s AÎ² peptide. Nature Computational Science, 2021, 1, 71-78.	3.8	42
8	Refinement of Î±-Synuclein Ensembles Against SAXS Data: Comparison of Force Fields and Methods. Frontiers in Molecular Biosciences, 2021, 8, 654333.	1.6	51
9	How to Determine Accurate Conformational Ensembles by Metadynamics Metainference: A Chignolin Study Case. Frontiers in Molecular Biosciences, 2021, 8, 694130.	1.6	5
10	Converging experimental and computational views of the knotting mechanism of a small knotted protein. Biophysical Journal, 2021, 120, 2276-2286.	0.2	12
11	High Conformational Flexibility of the E2F1/DP1/DNA Complex. Journal of Molecular Biology, 2021, 433, 167119.	2.0	4
12	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.	2.2	11
13	Structural Insight into IAPPâ€Derived Amyloid Inhibitors and Their Mechanism of Action. Angewandte Chemie - International Edition, 2020, 59, 5771-5781.	7.2	17
14	The dynamics of linear polyubiquitin. Science Advances, 2020, 6, .	4.7	38
15	Conformational Stability and Dynamics in Crystals Recapitulate Protein Behavior in Solution. Biophysical Journal, 2020, 119, 978-988.	0.2	3
16	Structural Basis of Inhibition of the Pioneer Transcription Factor NF-Y by Suramin. Cells, 2020, 9, 2370.	1.8	8
17	Small-molecule sequestration of amyloid-Î² as a drug discovery strategy for Alzheimerâ€™s disease. Science Advances, 2020, 6, .	4.7	95
18	Structural Insight into IAPPâ€Derived Amyloid Inhibitors and Their Mechanism of Action. Angewandte Chemie, 2020, 132, 5820-5830.	1.6	3

#	Article	IF	Citations
19	Determination of Protein Structural Ensembles by Hybrid-Resolution SAXS Restrained Molecular Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 2825-2834.	2.3	33
20	Mapping the transition state for a binding reaction between ancient intrinsically disordered proteins. Journal of Biological Chemistry, 2020, 295, 17698-17712.	1.6	12
21	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	9.0	655
22	Cryo-EM Structures of AzospirillumÂbrasilense Glutamate Synthase in Its Oligomeric Assemblies. Journal of Molecular Biology, 2019, 431, 4523-4526.	2.0	4
23	A structurally heterogeneous transition state underlies coupled binding and folding of disordered proteins. Journal of Biological Chemistry, 2019, 294, 1230-1239.	1.6	39
24	Probing Specificity in Disordered Protein Interactions with Small Molecules using Integrative Methods. Biophysical Journal, 2019, 116, 180a.	0.2	0
25	Cryo-EM structure of cardiac amyloid fibrils from an immunoglobulin light chain AL amyloidosis patient. Nature Communications, 2019, 10, 1269.	5.8	113
26	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.	1.5	8
27	Integrative Methods for Protein Dynamics and Aggregation. Biophysical Journal, 2019, 116, 50a.	0.2	0
28	A Practical Guide to the Simultaneous Determination of Protein Structure and Dynamics Using Metainference. Methods in Molecular Biology, 2019, 2022, 313-340.	0.4	3
29	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.	1.9	19
30	Conformational dynamics in crystals reveal the molecular bases for D76N beta-2 microglobulin aggregation propensity. Nature Communications, 2018, 9, 1658.	5.8	53
31	The Antibody Light-Chain Linker Regulates Domain Orientation and Amyloidogenicity. Journal of Molecular Biology, 2018, 430, 4925-4940.	2.0	27
32	Advanced simulation techniques for the thermodynamic and kinetic characterization of biological systems. Advances in Physics: X, 2018, 3, 1477531.	1.5	29
33	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.	3.3	39
34	An implementation of the maximum-caliber principle by replica-averaged time-resolved restrained simulations. Journal of Chemical Physics, 2018, 148, 184114.	1.2	16
35	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.	1.5	5
36	Structural basis for terminal loop recognition and stimulation of pri-miRNA-18a processing by hnRNP A1. Nature Communications, 2018, 9, 2479.	5.8	80

#	Article	IF	Citations
37	Determination of the conformational states of strychnine in solution using NMR residual dipolar couplings in a tensor-free approach. Methods, 2018, 148, 4-8.	1.9	13
38	Folding Mechanism of the SH3 Domain from Grb2. Journal of Physical Chemistry B, 2018, 122, 11166-11173.	1.2	9
39	MobiDB 3.0: more annotations for intrinsic disorder, conformational diversity and interactions in proteins. Nucleic Acids Research, 2018, 46, D471-D476.	6.5	190
40	Molecular dynamics ensemble refinement of the heterogeneous native state of NCBD using chemical shifts and NOEs. PeerJ, 2018, 6, e5125.	0.9	25
41	Principles of protein structural ensemble determination. Current Opinion in Structural Biology, 2017, 42, 106-116.	2.6	285
42	Networks of Dynamic Allostery Regulate Enzyme Function. Structure, 2017, 25, 276-286.	1.6	63
43	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.	6.6	18
44	Metadynamic metainference: Convergence towards force field independent structural ensembles of a disordered peptide. Journal of Chemical Physics, 2017, 146, 165102.	1.2	47
45	Structural Investigation of an Immunoglobulin Domain on the Ribosome using NMR Spectroscopy. Biophysical Journal, 2017, 112, 41a.	0.2	0
46	Characterization of Protein Kinase a Free Energy Landscape by NMR-Restrained Metadynamics. Biophysical Journal, 2017, 112, 50a.	0.2	1
47	Simultaneous quantification of protein order and disorder. Nature Chemical Biology, 2017, 13, 339-342.	3.9	113
48	Simultaneous NMR characterisation of multiple minima in the free energy landscape of an RNA UUCG tetraloop. Physical Chemistry Chemical Physics, 2017, 19, 2797-2804.	1.3	18
49	Integrative structural and dynamical biology with PLUMED-ISDB. Bioinformatics, 2017, 33, 3999-4000.	1.8	59
50	Sequence Specificity in the Entropy-Driven Binding of a Small Molecule and a Disordered Peptide. Journal of Molecular Biology, 2017, 429, 2772-2779.	2.0	62
51	The PHR Family: The Role of Extracellular Transglycosylases in Shaping Candida albicans Cells. Journal of Fungi (Basel, Switzerland), 2017, 3, 59.	1.5	21
52	Stabilization and structural analysis of a membrane-associated hIAPP aggregation intermediate. ELife, 2017, 6, .	2.8	61
53	Emergence and evolution of an interaction between intrinsically disordered proteins. ELife, 2017, 6, .	2.8	42
54	Rational design of mutations that change the aggregation rate of a protein while maintaining its native structure and stability. Scientific Reports, 2016, 6, 25559.	1.6	47

#	Article	IF	Citations
55	Towards a structural biology of the hydrophobic effect in protein folding. Scientific Reports, 2016, 6, 28285.	1.6	91
56	Properties of low-dimensional collective variables in the molecular dynamics of biopolymers. Physical Review E, 2016, 94, 052406.	0.8	4
57	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.	3.3	54
58	Identification and Structural Characterization of an Intermediate in the Folding of the Measles Virus X Domain. Journal of Biological Chemistry, 2016, 291, 10886-10892.	1.6	18
59	Molecular Recognition by Templated Folding of an Intrinsically Disordered Protein. Scientific Reports, 2016, 6, 21994.	1.6	87
60	Metadynamic metainference: Enhanced sampling of the metainference ensemble using metadynamics. Scientific Reports, 2016, 6, 31232.	1.6	76
61	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.	3.3	54
62	Metainference: A Bayesian inference method for heterogeneous systems. Science Advances, 2016, 2, e1501177.	4.7	180
63	A structural ensemble of a ribosomeâ€“nascent chain complex during cotranslational protein folding. Nature Structural and Molecular Biology, 2016, 23, 278-285.	3.6	135
64	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.	1.2	9
65	The inverted free energy landscape of an intrinsically disordered peptide by simulations and experiments. Scientific Reports, 2015, 5, 15449.	1.6	118
66	Mapping the Protein Fold Universe Using the CamTube Force Field in Molecular Dynamics Simulations. PLoS Computational Biology, 2015, 11, e1004435.	1.5	17
67	Dynamic binding mode of a Synaptotagmin-1â€“SNARE complex in solution. Nature Structural and Molecular Biology, 2015, 22, 555-564.	3.6	129
68	Using Pseudocontact Shifts and Residual Dipolar Couplings as Exact NMR Restraints for the Determination of Protein Structural Ensembles. Biochemistry, 2015, 54, 7470-7476.	1.2	19
69	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.	1.2	51
70	The H50Q Mutation Induces a 10-fold Decrease in the Solubility of Î±-Synuclein. Journal of Biological Chemistry, 2015, 290, 2395-2404.	1.6	65
71	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.	1.2	6
72	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.	1.6	15

#	Article	IF	Citations
73	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.	1.2	18
74	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.	2.0	77
75	Archaeal MBF1 binds to 30S and 70S ribosomes via its helixâ€“turnâ€“helix domain. Biochemical Journal, 2014, 462, 373-384.	1.7	16
76	The dynamics of interleukinâ€8 and its interaction with human CXC receptor I peptide. Protein Science, 2014, 23, 464-480.	3.1	21
77	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.	2.0	25
78	New opportunities for tensor-free calculations of residual dipolar couplings for the study of protein dynamics. Journal of Biomolecular NMR, 2014, 58, 233-238.	1.6	8
79	Conformational Recognition of an Intrinsically Disordered Protein. Biophysical Journal, 2014, 106, 1771-1779.	0.2	47
80	ALMOST: An all atom molecular simulation toolkit for protein structure determination. Journal of Computational Chemistry, 2014, 35, 1101-1105.	1.5	31
81	PLUMED 2: New feathers for an old bird. Computer Physics Communications, 2014, 185, 604-613.	3.0	2,454
82	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.	6.6	20
83	NMR characterization of the conformational fluctuations of the human lymphocyte functionâ€associated antigenâ€1 Iâ€domain. Protein Science, 2014, 23, 1596-1606.	3.1	8
84	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.	3.3	43
85	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.	2.3	6
86	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.	3.3	68
87	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.	0.2	0
88	MD Simulations of Intrinsically Disordered Proteins with Replica-Averaged Chemical Shift Restraints. Biophysical Journal, 2014, 106, 481a.	0.2	3
89	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.	0.2	0
90	Statistical Mechanics of the Denatured State of a Protein Using Replica-Averaged Metadynamics. Journal of the American Chemical Society, 2014, 136, 8982-8991.	6.6	69

#	Article	IF	Citations
91	Structural investigation of the folding of an immunoglobulin domain on the ribosome using NMR Spectroscopy (LB197). FASEB Journal, 2014, 28, LB197.	0.2	0
92	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.	1.2	13
93	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.	1.2	41
94	Thermodynamics of an Intrinsically Disordered Protein by Atomistic Simulations. Biophysical Journal, 2013, 104, 55a.	0.2	1
95	Molecular dynamics simulations with replica-averaged structural restraints generate structural ensembles according to the maximum entropy principle. Journal of Chemical Physics, 2013, 138, 094112.	1.2	169
96	Replica-Averaged Metadynamics. Journal of Chemical Theory and Computation, 2013, 9, 5610-5617.	2.3	64
97	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.	3.3	122
98	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.	1.1	89
99	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.	1.2	14
100	Ratcheted molecular-dynamics simulations identify efficiently the transition state of protein folding. Journal of Chemical Physics, 2012, 137, 235101.	1.2	24
101	Determination of Secondary Structure Populations in Disordered States of Proteins Using Nuclear Magnetic Resonance Chemical Shifts. Biochemistry, 2012, 51, 2224-2231.	1.2	316
102	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.	6.6	84
103	A Highly Compliant Protein Native State with a Spontaneous-like Mechanical Unfolding Pathway. Journal of the American Chemical Society, 2012, 134, 17068-17075.	6.6	29
104	Energy Landscape of the Prion Protein Helix 1 Probed by Metadynamics and NMR. Biophysical Journal, 2012, 102, 158-167.	0.2	39
105	Hierarchy of folding and unfolding events of protein G, CI2, and ACBP from explicit-solvent simulations. Journal of Chemical Physics, 2011, 134, 045105.	1.2	45
106	Identification of the folding inhibitors of hen-egg lysozyme: gathering the right tools. European Biophysics Journal, 2010, 39, 911-919.	1.2	2
107	Lymphotactin: How a protein can adopt two folds. Journal of Chemical Physics, 2009, 131, 245105.	1.2	22
108	PLUMED: A portable plugin for free-energy calculations with molecular dynamics. Computer Physics Communications, 2009, 180, 1961-1972.	3.0	1,448

#	Article	IF	Citations
109	Exploring the protein G helix freeâ€energy surface by solute tempering metadynamics. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1647-1654.	1.5	68
110	Early events in protein folding: Is there something more than hydrophobic burst?. Protein Science, 2008, 17, 1424-1433.	3.1	14
111	Urea and Guanidinium Chloride Denature Protein L in Different Ways in Molecular Dynamics Simulations. Biophysical Journal, 2008, 94, 4654-4661.	0.2	141
112	Atomistic Simulations of the HIV-1 Protease Folding Inhibition. Biophysical Journal, 2008, 95, 550-562.	0.2	12
113	Metadynamic sampling of the free-energy landscapes of proteins coupled with a Monte Carlo algorithm. Gene, 2008, 422, 37-40.	1.0	3
114	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.	3.3	59
115	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.	1.2	5