Andrea Cavalli

List of Publications by Year
in descending order

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41 papers	3,112 citations	304743 22 h-index	254184 43 g-index
49 all docs	49 docs citations	49 times ranked	3557 citing authors

#	Article	IF	Citations
1	Protein structure determination from NMR chemical shifts. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 9615-9620.	7.1	499
2	Structure of an Intermediate State in Protein Folding and Aggregation. Science, 2012, 336, 362-366.	12.6	339
3	Fast and Accurate Predictions of Protein NMR Chemical Shifts from Interatomic Distances. Journal of the American Chemical Society, 2009, 131, 13894-13895.	13.7	223
4	Prediction of aggregation rate and aggregation-prone segments in polypeptide sequences. Protein Science, 2005, 14, 2723-2734.	7.6	201
5	Metainference: A Bayesian inference method for heterogeneous systems. Science Advances, 2016, 2, e1501177.	10.3	180
6	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
7	Using NMR Chemical Shifts as Structural Restraints in Molecular Dynamics Simulations of Proteins. Structure, 2010, 18, 923-933.	3.3	141
8	Compartmentalized activities of the pyruvate dehydrogenase complex sustain lipogenesis in prostate cancer. Nature Genetics, 2018, 50, 219-228.	21.4	139
9	Dynamic binding mode of a Synaptotagmin-1â€“SNARE complex in solution. Nature Structural and Molecular Biology, 2015, 22, 555-564.	8.2	129
10	Recognition and inhibition of SARS-CoV-2 by humoral innate immunity pattern recognition molecules. Nature Immunology, 2022, 23, 275-286.	14.5	95
11	Structural Biology of STAT3 and Its Implications for Anticancer Therapies Development. International Journal of Molecular Sciences, 2018, 19, 1591.	4.1	92
12	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
13	CASD-NMR: critical assessment of automated structure determination by NMR. Nature Methods, 2009, 6, 625-626.	19.0	80
14	Blind Testing of Routine, Fully Automated Determination of Protein Structures from NMR Data. Structure, 2012, 20, 227-236.	3.3	75
15	Structure-based prediction of methyl chemical shifts in proteins. Journal of Biomolecular NMR, 2011, 50, 331-346.	2.8	65
16	Replica-Averaged Metadynamics. Journal of Chemical Theory and Computation, 2013, 9, 5610-5617.	5.3	64
17	Structure Determination of Proteinâ^'Protein Complexes Using NMR Chemical Shifts: Case of an Endonuclease Colicinâ^'Immunity Protein Complex. Journal of the American Chemical Society, 2008, 130, 15990-15996.	13.7	55
18	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

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19	Single or Multiple Access Channels to the CYP450s Active Site? An Answer from Free Energy Simulations of the Human Aromatase Enzyme. Journal of Physical Chemistry Letters, 2017, 8, 2036-2042.	4.6	41
20	Probabilistic Determination of Native State Ensembles of Proteins. Journal of Chemical Theory and Computation, 2014, 10, 3484-3491.	5.3	38
21	ALMOST: An all atom molecular simulation toolkit for protein structure determination. Journal of Computational Chemistry, 2014, 35, 1101-1105.	3.3	31
22	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
23	Protein Tunnels: The Case of Urease Accessory Proteins. Journal of Chemical Theory and Computation, 2017, 13, 2322-2331.	5.3	25
24	Compounds targeting OSBPL7 increase ABCA1-dependent cholesterol efflux preserving kidney function in two models of kidney disease. Nature Communications, 2021, 12, 4662.	12.8	24
25	Molecular Dynamics of Biomolecules through Direct Analysis of Dipolar Couplings. Journal of the American Chemical Society, 2015, 137, 6270-6278.	13.7	23
26	Machine learning analyses of antibody somatic mutations predict immunoglobulin light chain toxicity. Nature Communications, 2021, 12, 3532.	12.8	23
27	Using Sideâ€€Chain Aromatic Proton Chemical Shifts for a Quantitative Analysis of Protein Structures. Angewandte Chemie - International Edition, 2011, 50, 9620-9623.	13.8	20
28	The Dynamic Basis for Signal Propagation in Human Pin1-WW. Structure, 2016, 24, 1464-1475.	3.3	20
29	Oxidation State Dependent Conformational Changes of HMGB1 Regulate the Formation of the CXCL12/HMGB1 Heterocomplex. Computational and Structural Biotechnology Journal, 2019, 17, 886-894.	4.1	20
30	How phosphorylation influences E1 subunit pyruvate dehydrogenase: A computational study. Scientific Reports, 2018, 8, 14683.	3.3	17
31	EZH2-induced lysine K362 methylation enhances TMPRSS2-ERG oncogenic activity in prostate cancer. Nature Communications, 2021, 12, 4147.	12.8	17
32	Archaeal MBF1 binds to 30S and 70S ribosomes via its helixâ€“turnâ€“helix domain. Biochemical Journal, 2014, 462, 373-384.	3.7	16
33	Using Chemical Shifts to Determine Structural Changes in Proteins upon Complex Formation. Journal of Physical Chemistry B, 2011, 115, 9491-9494.	2.6	15
34	Characterization of the Conformational Fluctuations in the Josephin Domain of Ataxin-3. Biophysical Journal, 2014, 107, 2932-2940.	0.5	15
35	Molecular Determinants for Unphosphorylated STAT3 Dimerization Determined by Integrative Modeling. Biochemistry, 2015, 54, 5489-5501.	2.5	15
36	Zinc(<scp>ii</scp>)-mediated diastereoselective Passerini reactions of biocatalytically desymmetrised renewable inputs. Organic Chemistry Frontiers, 2020, 7, 380-398.	4.5	14

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37	Insights into the coiled-coil organization of the Hendra virus phosphoprotein from combined biochemical and SAXS studies. Virology, 2015, 477, 42-55.	2.4	12
38	Systematic Development of Peptide Inhibitors Targeting the CXCL12/HMGB1 Interaction. Journal of Medicinal Chemistry, 2021, 64, 13439-13450.	6.4	8
39	Analysis of the performance of the CHESHIRE and YAPP methods at CASD-NMR round 3. Journal of Biomolecular NMR, 2015, 62, 503-509.	2.8	6
40	Enhancing coevolution-based contact prediction by imposing structural self-consistency of the contacts. Scientific Reports, 2018, 8, 11112.	3.3	3
41	Computational Identification of a Putative Allosteric Binding Pocket in TMPRSS2. Frontiers in Molecular Biosciences, 2021, 8, 666626.	3.5	3