Alessandro Cembran

List of Publications by Year
in descending order

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56 papers	2,461 citations	218381 26 h-index	233125 45 g-index
57 all docs	57 docs citations	57 times ranked	3137 citing authors

#	Article	IF	Citations
1	Insight From Animals Resistant to Prion Diseases: Deciphering the Genotype â€“ Morphotype â€“ Phenotype Code for the Prion Protein. Frontiers in Cellular Neuroscience, 2020, 14, 254.	1.8	12
2	Mechanical Unfolding of Spectrin Repeats Induces Water-Molecule Ordering. Biophysical Journal, 2020, 118, 1076-1089.	0.2	3
3	FRET Analysis of Ionic Strength Sensors in the Hofmeister Series of Salt Solutions Using Fluorescence Lifetime Measurements. Journal of Physical Chemistry B, 2020, 124, 3447-3458.	1.2	12
4	Atomic-Level Characterization of the Structural Dynamics of Azurin Variants with Tuned Reduction Potentials. Biophysical Journal, 2018, 114, 521a.	0.2	0
5	The Role of Hydrophobic Interactions and Water Dynamics Around Dystrophin Spectrin Repeats. Biophysical Journal, 2018, 114, 525a.	0.2	0
6	Dynamics of Dystrophinâ€™s Actin-Binding Domain. Biophysical Journal, 2018, 115, 445-454.	0.2	8
7	Tuning Sulfur Oxidation States on Thioetherâ€Bridged Peptide Macrocycles for Modulation of Protein Interactions. ChemBioChem, 2017, 18, 1836-1844.	1.3	18
8	Spectroscopic and Computational Analysis of Dystrophin Regulation of Actin Dynamics. Biophysical Journal, 2016, 110, 128a.	0.2	0
9	Molecular Dynamics Simulation and Markov State Model Reveal Irregular Metastable Conformation and Allostery In DNAJB-PKAc. Biophysical Journal, 2016, 110, 51a-52a.	0.2	0
10	Oxidation increases the strength of the methionine-aromatic interaction. Nature Chemical Biology, 2016, 12, 860-866.	3.9	53
11	Hydrophobic Interactions Elicit Cooperative Response in Dystrophin. Biophysical Journal, 2016, 110, 362a.	0.2	0
12	Sarcolipin-Mediated Regulation of SERCA by Computer Simulations. Biophysical Journal, 2015, 108, 384a.	0.2	0
13	Dysfunctional Conformational Dynamics of Protein Kinase a from R14 Deletion of Phospholamban. Biophysical Journal, 2015, 108, 529a.	0.2	0
14	Oxidation Increases the Strength of the Methionine-Aromatic Interaction. Biophysical Journal, 2015, 108, 17a.	0.2	0
15	Dysfunctional conformational dynamics of protein kinase A induced by a lethal mutant of phospholamban hinder phosphorylation. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 3716-3721.	3.3	43
16	Synchronous Opening and Closing Motions Are Essential for cAMP-Dependent Protein Kinase A Signaling. Structure, 2014, 22, 1735-1743.	1.6	55
17	Solid-State NMR Structures of Phospholamban or Sarcolipin Bound to Calcium ATPase (SERCA) Reveal the Mode of Inhibition. Biophysical Journal, 2014, 106, 585a.	0.2	0
18	Quantitative Interpretation of Chemical Shifts Enables Mapping Proteins Conformational Landscape. Biophysical Journal, 2014, 106, 807a.	0.2	0

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19	NMR mapping of protein conformational landscapes using coordinated behavior of chemical shifts upon ligand binding. Physical Chemistry Chemical Physics, 2014, 16, 6508-6518.	1.3	54
20	Investigating the role of a backbone to substrate hydrogen bond in OMP decarboxylase using a site-specific amide to ester substitution. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 15066-15071.	3.3	15
21	Connecting Protein Conformational Dynamics with Catalytic Function As Illustrated in Dihydrofolate Reductase. Biochemistry, 2013, 52, 2036-2049.	1.2	70
22	Concerted Hydrogen Atom and Electron Transfer Mechanism for Catalysis by Lysine-Specific Demethylase. Journal of Physical Chemistry B, 2013, 117, 8422-8429.	1.2	15
23	Role of conformational entropy in the activity and regulation of the catalytic subunit of protein kinase <scp>A</scp>. FEBS Journal, 2013, 280, 5608-5615.	2.2	21
24	Conformational Equilibrium of N-Myristoylated cAMP-Dependent Protein Kinase A by Molecular Dynamics Simulations. Biochemistry, 2012, 51, 10186-10196.	1.2	27
25	Multilevel X-Pol: A Fragment-Based Method with Mixed Quantum Mechanical Representations of Different Fragments. Journal of Physical Chemistry B, 2012, 116, 6781-6788.	1.2	32
26	The Third Dimension of a More Oâ€™Ferrallâ€“Jencks Diagram for Hydrogen Atom Transfer in the Isoelectronic Hydrogen Exchange Reactions of (PhX)₂H^{â€¢} with X = O, NH, and CH₂. Journal of Chemical Theory and Computation, 2012, 8, 4347-4358.	2.3	30
27	The Methionine-aromatic Motif Plays a Unique Role in Stabilizing Protein Structure. Journal of Biological Chemistry, 2012, 287, 34979-34991.	1.6	261
28	Allostery and Binding Cooperativity of the Catalytic Subunit of Protein Kinase A by NMR Spectroscopy and Molecular Dynamics Simulations. Advances in Protein Chemistry and Structural Biology, 2012, 87, 363-389.	1.0	41
29	Flickering dipoles in the gas phase: Structures, internal dynamics, and dipole moments of Î²-naphthol-H2O in its ground and excited electronic states. Journal of Chemical Physics, 2011, 134, 114304.	1.2	9
30	Generalized X-Pol Theory and Charge Delocalization States. Journal of Chemical Theory and Computation, 2010, 6, 2402-2410.	2.3	26
31	A Non-Orthogonal Block-Localized Effective Hamiltonian Approach for Chemical and Enzymatic Reactions. Journal of Chemical Theory and Computation, 2010, 6, 2242-2251.	2.3	18
32	On the Interfragment Exchange in the X-Pol Method. Journal of Chemical Theory and Computation, 2010, 6, 2469-2476.	2.3	27
33	Internal Dynamics of an Analytically Coarse-Grained Protein. Journal of Chemical Theory and Computation, 2010, 6, 3601-3612.	2.3	4
34	Aborted double bicycle-pedal isomerization with hydrogen bond breaking is the primary event of bacteriorhodopsin proton pumping. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 20172-20177.	3.3	88
35	A refinement protocol to determine structure, topology, and depth of insertion of membrane proteins using hybrid solution and solid-state NMR restraints. Journal of Biomolecular NMR, 2009, 44, 195-205.	1.6	48
36	Block-Localized Density Functional Theory (BLDFT), Diabatic Coupling, and Their Use in Valence Bond Theory for Representing Reactive Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2009, 5, 2702-2716.	2.3	110

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37	Tilt and Azimuthal Angles of a Transmembrane Peptide: A Comparison between Molecular Dynamics Calculations and Solid-State NMR Data of Sarcolipin in Lipid Membranes. Biophysical Journal, 2009, 96, 3648-3662.	0.2	33
38	On the Function of Pentameric Phospholamban: Ion Channel or Storage Form?. Biophysical Journal, 2009, 96, L60-L62.	0.2	38
39	Kinetic Isotope Effects from Hybrid Classical and Quantum Path Integral Computations. RSC Biomolecular Sciences, 2009, , 105-131.	0.4	5
40	Controlling the Inhibition of the Sarcoplasmic Ca2+-ATPase by Tuning Phospholamban Structural Dynamics. Journal of Biological Chemistry, 2007, 282, 37205-37214.	1.6	55
41	About the intrinsic photochemical properties of the 11-cis retinal chromophore: computational clues for a trap state and a lever effect in Rhodopsin catalysis. Theoretical Chemistry Accounts, 2007, 118, 173-183.	0.5	32
42	Potential energy functions for an intramolecular proton transfer reaction in the ground and excited state. Theoretical Chemistry Accounts, 2007, 118, 211-218.	0.5	8
43	Excited state intramolecular proton transfer in 1-(trifluoroacetylamino)naphthaquinone: a CASPT2//CASSCF computational study. Molecular Physics, 2006, 104, 943-955.	0.8	8
44	From The Cover: The retinal chromophore/chloride ion pair: Structure of the photoisomerization path and interplay of charge transfer and covalent states. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6255-6260.	3.3	108
45	Computation of Photochemical Reaction Mechanisms in Organic Chemistry. Theoretical and Computational Chemistry, 2005, 16, 191-223.	0.2	9
46	Structure, Spectroscopy, and Spectral Tuning of the Gas-Phase Retinal Chromophore:â€‰ The Î²-Ionone â€œHandleâ€•and Alkyl Group Effect. Journal of Physical Chemistry A, 2005, 109, 6597-6605.	1.1	83
47	On the Mechanism of the cisâ^'trans Isomerization in the Lowest Electronic States of Azobenzene:â€‰ S0, S1, and T1. Journal of the American Chemical Society, 2004, 126, 3234-3243.	6.6	431
48	A theoretical study of the lowest electronic states of azobenzene: the role of torsion coordinate in the cisâ€“trans photoisomerization. Theoretical Chemistry Accounts, 2004, 111, 363-372.	0.5	131
49	Complete-active-space self-consistent-field/Amber parameterization of the Lys296?retinal?Glu113 rhodopsin chromophore-counterion system. Theoretical Chemistry Accounts, 2004, 112, 335.	0.5	63
50	Structure of the intersection space associated with Z/E photoisomerization of retinal in rhodopsin proteins. Faraday Discussions, 2004, 127, 179-191.	1.6	60
51	Counterion Controlled Photoisomerization of Retinal Chromophore Models:Â a Computational Investigation. Journal of the American Chemical Society, 2004, 126, 16018-16037.	6.6	89
52	Structure of the Conical Intersections Driving the cisâ€”trans Photoisomerization of Conjugated Molecules. ChemInform, 2003, 34, no.	0.1	0
53	Excited-State Singlet Manifold and Oscillatory Features of a Nonatetraeniminium Retinal Chromophore Model. Journal of the American Chemical Society, 2003, 125, 12509-12519.	6.6	41
54	Structure of the Conical Intersections Driving the cisâ€“trans Photoisomerization of Conjugated MoleculesÂ¶. Photochemistry and Photobiology, 2002, 76, 622.	1.3	91

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55	Retinal chromophore photoinduced molecular motion and reactivity: isolated conditions and counterion effects. Journal of Computational Methods in Sciences and Engineering, 2002, 2, 431-439.	0.1	0
56	Cyclooctatetraene Computational Photo- and Thermal Chemistry:Â A Reactivity Model for Conjugated Hydrocarbons. Journal of the American Chemical Society, 2002, 124, 13770-13789.	6.6	75