Luciano A Abriata

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	How Technologies Assisted Science Learning at Home During the COVID-19 Pandemic. DNA and Cell Biology, 2022, 41, 19-24.	0.9	9
2	Online tools to easily build virtual molecular models for display in augmented and virtual reality on the web. Journal of Molecular Graphics and Modelling, 2022, 114, 108164.	1.3	20
3	State-of-the-art web services for <i>de novo</i> protein structure prediction. Briefings in Bioinformatics, 2021, 22, .	3.2	13
4	Site‧pecific Phosphorylation of Huntingtin Exonâ€1 Recombinant Proteins Enabled by the Discovery of Novel Kinases. ChemBioChem, 2021, 22, 217-231.	1.3	18
5	Bottom-up de novo design of functional proteins with complex structural features. Nature Chemical Biology, 2021, 17, 492-500.	3.9	65
6	Assessment of transferable forcefields for protein simulations attests improved description of disordered states and secondary structure propensities, and hints at multi-protein systems as the next challenge for optimization. Computational and Structural Biotechnology Journal, 2021, 19, 2626-2636.	1.9	25
7	Inositol pyrophosphates promote the interaction of SPX domains with the coiled-coil motif of PHR transcription factors to regulate plant phosphate homeostasis. Nature Communications, 2021, 12, 384.	5.8	105
8	A minimalistic cyclic ice-binding peptide from phage display. Nature Communications, 2021, 12, 2675.	5.8	26
9	3D architecture and structural flexibility revealed in the subfamily of large glutamate dehydrogenases by a mycobacterial enzyme. Communications Biology, 2021, 4, 684.	2.0	3
10	MoleculARweb: A Web Site for Chemistry and Structural Biology Education through Interactive Augmented Reality out of the Box in Commodity Devices. Journal of Chemical Education, 2021, 98, 2243-2255.	1.1	26
11	Reviewing Challenges of Predicting Protein Melting Temperature Change Upon Mutation Through the Full Analysis of a Highly Detailed Dataset with High-Resolution Structures. Molecular Biotechnology, 2021, 63, 863-884.	1.3	13
12	Investigating Crosstalk Among PTMs Provides Novel Insight Into the Structural Basis Underlying the Differential Effects of Nt17 PTMs on Mutant Httex1 Aggregation. Frontiers in Molecular Biosciences, 2021, 8, 686086.	1.6	8
13	Democratizing interactive, immersive experiences for science education with WebXR. Nature Computational Science, 2021, 1, 631-632.	3.8	13
14	S-acylation controls SARS-CoV-2 membrane lipid organization and enhances infectivity. Developmental Cell, 2021, 56, 2790-2807.e8.	3.1	80
15	Control and Characterization of the Compactness of Single-Chain Nanoparticles. Macromolecules, 2021, 54, 11459-11467.	2.2	11
16	Structural and DNA binding properties of mycobacterial integration host factor mIHF. Journal of Structural Biology, 2020, 209, 107434.	1.3	3
17	Ligand Binding to the Collagen VI Receptor Triggers a Talin-to-RhoA Switch that Regulates Receptor Endocytosis. Developmental Cell, 2020, 53, 418-430.e4.	3.1	12
18	Building blocks for commodity augmented reality-based molecular visualization and modeling in web browsers. PeerJ Computer Science, 2020, 6, e260.	2.7	13

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19	De novo development of proteolytically resistant therapeutic peptides for oral administration. Nature Biomedical Engineering, 2020, 4, 560-571.	11.6	65
20	De novo protein design enables the precise induction of RSV-neutralizing antibodies. Science, 2020, 368, .	6.0	137
21	Will Cryo-Electron Microscopy Shift the Current Paradigm in Protein Structure Prediction?. Journal of Chemical Information and Modeling, 2020, 60, 2443-2447.	2.5	8
22	About the need to make computational models of biological macromolecules available and discoverable. Bioinformatics, 2020, 36, 2952-2954.	1.8	7
23	Computational Tools for Structural Analysis of Proteins. , 2019, , 539-549.		Ο
24	A further leap of improvement in tertiary structure prediction in CASP13 prompts new routes for future assessments. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1100-1112.	1.5	73
25	Population Structure, Molecular Epidemiology, and β-Lactamase Diversity among Stenotrophomonas maltophilia Isolates in the United States. MBio, 2019, 10, .	1.8	52
26	pH-Induced Binding of the Axial Ligand in an Engineered Cu _A Site Favors the I€ _u State. Inorganic Chemistry, 2019, 58, 15687-15691.	1.9	0
27	Active Site-Induced Evolutionary Constraints Follow Fold Polarity Principles in Soluble Globular Enzymes. Molecular Biology and Evolution, 2019, 36, 1728-1733.	3.5	7
28	An experiment-informed signal transduction model for the role of the Staphylococcus aureus MecR1 protein in β-lactam resistance. Scientific Reports, 2019, 9, 19558.	1.6	11
29	Transmembrane Prolines Mediate Signal Sensing and Decoding in Bacillus subtilis DesK Histidine Kinase. MBio, 2019, 10, .	1.8	21
30	Nucleo-cytosolic Shuttling of ARGONAUTE1 Prompts a Revised Model of the Plant MicroRNA Pathway. Molecular Cell, 2018, 69, 709-719.e5.	4.5	193
31	Augmenting Research, Education, and Outreach with Client-Side Web Programming. Trends in Biotechnology, 2018, 36, 473-476.	4.9	13
32	Assessment of dataâ€assisted prediction by inclusion of crosslinking/massâ€spectrometry and small angle Xâ€ray scattering data in the 12 th Critical Assessment of protein Structure Prediction experiment. Proteins: Structure, Function and Bioinformatics, 2018, 86, 215-227.	1.5	4
33	Electron transfer in an acidophilic bacterium: interaction between a diheme cytochrome and a cupredoxin. Chemical Science, 2018, 9, 4879-4891.	3.7	17
34	Definition and classification of evaluation units for tertiary structure prediction in CASP12 facilitated through semiâ€automated metrics. Proteins: Structure, Function and Bioinformatics, 2018, 86, 16-26.	1.5	12
35	Mitochondrial cytochrome c oxidase biogenesis: Recent developments. Seminars in Cell and Developmental Biology, 2018, 76, 163-178.	2.3	225
36	Assessment of hard target modeling in CASP12 reveals an emerging role of alignmentâ€based contact prediction methods. Proteins: Structure, Function and Bioinformatics, 2018, 86, 97-112.	1.5	79

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37	Structural database resources for biological macromolecules. Briefings in Bioinformatics, 2017, 18, bbw049.	3.2	13
38	Signal Sensing and Transduction by Histidine Kinases as Unveiled through Studies on a Temperature Sensor. Accounts of Chemical Research, 2017, 50, 1359-1366.	7.6	46
39	Structural, physicochemical and dynamic features conserved within the aerolysin pore-forming toxin family. Scientific Reports, 2017, 7, 13932.	1.6	38
40	Functional assays for the assessment of the pathogenicity of variants in GOSR2, an ER-to-Golgi SNARE involved in progressive myoclonus epilepsies. DMM Disease Models and Mechanisms, 2017, 10, 1391-1398.	1.2	11
41	Web Apps Come of Age for Molecular Sciences. Informatics, 2017, 4, 28.	2.4	20
42	Detection and sequence/structure mapping of biophysical constraints to protein variation in saturated mutational libraries and protein sequence alignments with a dedicated server. BMC Bioinformatics, 2016, 17, 242.	1.2	18
43	Immobilization of the N-terminal helix stabilizes prefusion paramyxovirus fusion proteins. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E3844-51.	3.3	4
44	Molecular Effects of Concentrated Solutes on Protein Hydration, Dynamics, and Electrostatics. Biophysical Journal, 2016, 111, 743-755.	0.2	29
45	Optimization of Conformational Dynamics in an Epistatic Evolutionary Trajectory. Molecular Biology and Evolution, 2016, 33, 1768-1776.	3.5	51
46	A coiled coil switch mediates cold sensing by the thermosensory protein <scp>DesK</scp> . Molecular Microbiology, 2015, 98, 258-271.	1.2	50
47	Reversible Switching of Redoxâ€Active Molecular Orbitals and Electron Transfer Pathways in Cu _A Sites of Cytochromeâ€ <i>c</i> Oxidase. Angewandte Chemie - International Edition, 2015, 54, 9555-9559.	7.2	11
48	How Structural and Physicochemical Determinants Shape Sequence Constraints in a Functional Enzyme. PLoS ONE, 2015, 10, e0118684.	1.1	41
49	Assessing the potential of atomistic molecular dynamics simulations to probe reversible protein-protein recognition and binding. Scientific Reports, 2015, 5, 10549.	1.6	50
50	The importance of dynamics in integrative modeling of supramolecular assemblies. Current Opinion in Structural Biology, 2015, 31, 28-34.	2.6	20
51	GtrA Protein Rv3789 Is Required for Arabinosylation of Arabinogalactan in Mycobacterium tuberculosis. Journal of Bacteriology, 2015, 197, 3686-3697.	1.0	26
52	Redox-state sensing by hydrogen bonds in the CuA center of cytochrome c oxidase. Journal of Inorganic Biochemistry, 2014, 132, 18-20.	1.5	5
53	Molecular dynamics simulations of apocupredoxins: insights into the formation and stabilization of copper sites under entatic control. Journal of Biological Inorganic Chemistry, 2014, 19, 565-575.	1.1	19
54	Control of the Electronic Ground State on an Electronâ€Transfer Copper Site by Secondâ€Sphere Perturbations. Angewandte Chemie - International Edition, 2014, 53, 6188-6192.	7.2	18

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55	Dissecting the Effects of Concentrated Carbohydrate Solutions on Protein Diffusion, Hydration, and Internal Dynamics. Journal of Physical Chemistry B, 2014, 118, 5310-5321.	1.2	24
56	A dimerization interface mediated by functionally critical residues creates interfacial disulfide bonds and copper sites in CueP. Journal of Inorganic Biochemistry, 2014, 140, 199-201.	1.5	5
57	All-atom simulations of crowding effects on ubiquitin dynamics. Physical Biology, 2013, 10, 045006.	0.8	13
58	Native CuA redox sites are largely resilient to pH variations within a physiological range. Chemical Communications, 2013, 49, 5381.	2.2	18
59	Investigation of non-corrin cobalt(II)-containing sites in protein structures of the Protein Data Bank. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2013, 69, 176-183.	0.5	6
60	Off-the-Vine Ripening of Tomato Fruit Causes Alteration in the Primary Metabolite Composition. Metabolites, 2013, 3, 967-978.	1.3	37
61	Investigation of non-corrin cobalt(II)-containing sites in protein structures of the Protein Data Bank. Acta Crystallographica Section B: Structural Science, 2013, 69, 176-183.	1.8	0
62	Flexibility of the metal-binding region in apo-cupredoxins. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 9254-9259.	3.3	67
63	Analysis of copper–ligand bond lengths in X-ray structures of different types of copper sites in proteins. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 1223-1231.	2.5	21
64	Sequence–function–stability relationships in proteins from datasets of functionally annotated variants: The case of TEM Î²â€łactamases. FEBS Letters, 2012, 586, 3330-3335.	1.3	24
65	Alternative ground states enable pathway switching in biological electron transfer. Proceedings of the United States of America, 2012, 109, 17348-17353.	3.3	31
66	Utilization of NMR spectroscopy to study biological fluids and metabolic processes: Two introductory activities. Concepts in Magnetic Resonance Part A: Bridging Education and Research, 2012, 40A, 171-178.	0.2	18
67	A Simple Spreadsheet Program To Simulate and Analyze the Far-UV Circular Dichroism Spectra of Proteins. Journal of Chemical Education, 2011, 88, 1268-1273.	1.1	22
68	Electronic Structure of the Ground and Excited States of the CuA Site by NMR Spectroscopy. Journal of the American Chemical Society, 2009, 131, 1939-1946.	6.6	47
69	Mechanism of CuA assembly. Nature Chemical Biology, 2008, 4, 599-601.	3.9	113
70	Engineered Mononuclear Variants in Bacillus cereus Metallo-β-lactamase BcII Are Inactive. Biochemistry, 2008, 47, 8590-8599.	1.2	25