Elena Papaleo

List of Publications by Year
in descending order

119 papers	4,707 citations	117571 34 h-index	133188 59 g-index
143 all docs	143 docs citations	143 times ranked	6910 citing authors

#	Article	IF	Citations
1	New functionalities in the TCGAbiolinks package for the study and integration of cancer data from GDC and GTEx. PLoS Computational Biology, 2019, 15, e1006701.	1.5	319
2	The Role of Protein Loops and Linkers in Conformational Dynamics and Allostery. Chemical Reviews, 2016, 116, 6391-6423.	23.0	302
3	Free-energy landscape, principal component analysis, and structural clustering to identify representative conformations from molecular dynamics simulations: The myoglobin case. Journal of Molecular Graphics and Modelling, 2009, 27, 889-899.	1.3	298
4	HUWE1 E3 ligase promotes PINK1/PARKIN-independent mitophagy by regulating AMBRA1 activation via IKKÎ±. Nature Communications, 2018, 9, 3755.	5.8	198
5	DisProt: intrinsic protein disorder annotation in 2020. Nucleic Acids Research, 2020, 48, D269-D276.	6.5	141
6	Protein aggregation: Mechanisms and functional consequences. International Journal of Biochemistry and Cell Biology, 2012, 44, 1541-1554.	1.2	139
7	DisProt in 2022: improved quality and accessibility of protein intrinsic disorder annotation. Nucleic Acids Research, 2022, 50, D480-D487.	6.5	117
8	An Efficient Method for Estimating the Hydrodynamic Radius of Disordered Protein Conformations. Biophysical Journal, 2017, 113, 550-557.	0.2	110
9	PyInteraph: A Framework for the Analysis of Interaction Networks in Structural Ensembles of Proteins. Journal of Chemical Information and Modeling, 2014, 54, 1537-1551.	2.5	107
10	Predicting the impact of Lynch syndrome-causing missense mutations from structural calculations. PLoS Genetics, 2017, 13, e1006739.	1.5	90
11	Comparing Molecular Dynamics Force Fields in the Essential Subspace. PLoS ONE, 2015, 10, e0121114.	1.1	80
12	ETHE1 mutations are specific to ethylmalonic encephalopathy. Journal of Medical Genetics, 2005, 43, 340-346.	1.5	78
13	Flexibility and enzymatic cold-adaptation: A comparative molecular dynamics investigation of the elastase family. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2006, 1764, 1397-1406.	1.1	70
14	An optimal distance cutoff for contact-based Protein Structure Networks using side-chain centers of mass. Scientific Reports, 2017, 7, 2838.	1.6	70
15	Interpreting pathways to discover cancer driver genes with Moonlight. Nature Communications, 2020, 11, 69.	5.8	66
16	xPyder: A PyMOL Plugin To Analyze Coupled Residues and Their Networks in Protein Structures.. Journal of Chemical Information and Modeling, 2012, 52, 1865-1874.	2.5	64
17	Integrating atomistic molecular dynamics simulations, experiments, and network analysis to study protein dynamics: strength in unity. Frontiers in Molecular Biosciences, 2015, 2, 28.	1.6	64
18	ENCORE: Software for Quantitative Ensemble Comparison. PLoS Computational Biology, 2015, 11, e1004415.	1.5	64

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19	Mapping transiently formed and sparsely populated conformations on a complex energy landscape. ELife, 2016, 5, .	2.8	63
20	Compaction Properties of an Intrinsically Disordered Protein: Sic1 and Its Kinase-Inhibitor Domain. Biophysical Journal, 2011, 100, 2243-2252.	0.2	62
21	How well do force fields capture the strength of salt bridges in proteins?. PeerJ, 2018, 6, e4967.	0.9	58
22	Mutations of C19orf12, coding for a transmembrane glycine zipper containing mitochondrial protein, cause mis-localization of the protein, inability to respond to oxidative stress and increased mitochondrial Ca2+. Frontiers in Genetics, 2015, 6, 185.	1.1	57
23	Toward mechanistic models for genotypeâ€“phenotype correlations in phenylketonuria using protein stability calculations. Human Mutation, 2019, 40, 444-457.	1.1	56
24	Protein flexibility in psychrophilic and mesophilic trypsins. Evidence of evolutionary conservation of protein dynamics in trypsinâ€like serineâ€proteases. FEBS Letters, 2008, 582, 1008-1018.	1.3	53
25	Dynamic properties of extremophilic subtilisin-like serine-proteases. Journal of Structural Biology, 2011, 174, 69-83.	1.3	52
26	A combined computational and structural model of the full-length human prolactin receptor. Nature Communications, 2016, 7, 11578.	5.8	52
27	Computational and cellular studies reveal structural destabilization and degradation of MLH1 variants in Lynch syndrome. ELife, 2019, 8, .	2.8	49
28	Cytokine profiling of tumor interstitial fluid of the breast and its relationship with lymphocyte infiltration and clinicopathological characteristics. OncoImmunology, 2016, 5, e1248015.	2.1	48
29	Conformational Changes and Free Energies in a Proline Isomerase. Journal of Chemical Theory and Computation, 2014, 10, 4169-4174.	2.3	46
30	The human Na+/H+ exchanger 1 is a membrane scaffold protein for extracellular signal-regulated kinase 2. BMC Biology, 2016, 14, 31.	1.7	45
31	Molecular Determinants of Enzyme Cold Adaptation: Comparative Structural and Computational Studies of Cold- and Warm-Adapted Enzymes. Current Protein and Peptide Science, 2011, 12, 657-683.	0.7	44
32	E2 superfamily of ubiquitin-conjugating enzymes: constitutively active or activated through phosphorylation in the catalytic cleft. Scientific Reports, 2015, 5, 14849.	1.6	43
33	Alterations of the interactome of Bcl-2 proteins in breast cancer at the transcriptional, mutational and structural level. PLoS Computational Biology, 2019, 15, e1007485.	1.5	42
34	Mechanisms of Intramolecular Communication in a Hyperthermophilic Acylaminoacyl Peptidase: A Molecular Dynamics Investigation. PLoS ONE, 2012, 7, e35686.	1.1	40
35	Communication Routes in ARID Domains between Distal Residues in Helix 5 and the DNA-Binding Loops. PLoS Computational Biology, 2014, 10, e1003744.	1.5	40
36	DNA-binding protects p53 from interactions with cofactors involved in transcription-independent functions. Nucleic Acids Research, 2016, 44, gkw770.	6.5	40

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37	The role of salt bridges on the temperature adaptation of aqualysin I, a thermostable subtilisin-like proteinase. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 2174-2181.	1.1	39
38	Optimization of electrostatics as a strategy for cold-adaptation: A case study of cold- and warm-active elastases. Journal of Molecular Graphics and Modelling, 2007, 26, 93-103.	1.3	38
39	Molecular Dynamics of Mesophilic-Like Mutants of a Cold-Adapted Enzyme: Insights into Distal Effects Induced by the Mutations. PLoS ONE, 2011, 6, e24214.	1.1	38
40	MIR7â€“3HG, a MYC-dependent modulator of cell proliferation, inhibits autophagy by a regulatory loop involving AMBRA1. Autophagy, 2017, 13, 554-566.	4.3	38
41	Evidence for the Formation of a Moâ€“H Intermediate in the Catalytic Cycle of Formate Dehydrogenase. Inorganic Chemistry, 2012, 51, 8331-8339.	1.9	37
42	Effects of Calcium Binding on Structure and Autolysis Regulation in Trypsins. A Molecular Dynamics Investigation. Journal of Chemical Theory and Computation, 2005, 1, 1286-1297.	2.3	35
43	Molecular dynamics-guided discovery of an ago-allosteric modulator for GPR40/FFAR1. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 7123-7128.	3.3	35
44	The Mutational Landscape of the Oncogenic MZF1 SCAN Domain in Cancer. Frontiers in Molecular Biosciences, 2016, 3, 78.	1.6	34
45	A phosphorylation-motif for tuneable helix stabilisation in intrinsically disordered proteins â€“ Lessons from the sodium proton exchanger 1 (NHE1). Cellular Signalling, 2017, 37, 40-51.	1.7	34
46	Distinct signatures of lung cancer types: aberrant mucin O-glycosylation and compromised immune response. BMC Cancer, 2019, 19, 824.	1.1	34
47	Paths of long-range communication in the E2 enzymes of family 3: a molecular dynamics investigation. Physical Chemistry Chemical Physics, 2012, 14, 12515.	1.3	33
48	Computational Structural Biology of S-nitrosylation of Cancer Targets. Frontiers in Oncology, 2018, 8, 272.	1.3	32
49	A comparative study of cold- and warm-adapted Endonucleases A using sequence analyses and molecular dynamics simulations. PLoS ONE, 2017, 12, e0169586.	1.1	30
50	Validation of protein models by a neural network approach. BMC Bioinformatics, 2008, 9, 66.	1.2	29
51	An Acidic Loop and Cognate Phosphorylation Sites Define a Molecular Switch That Modulates Ubiquitin Charging Activity in Cdc34-Like Enzymes. PLoS Computational Biology, 2011, 7, e1002056.	1.5	29
52	Secreted breast tumor interstitial fluid microRNAs and their target genes are associated with triple-negative breast cancer, tumor grade, and immune infiltration. Breast Cancer Research, 2020, 22, 73.	2.2	29
53	Relevance of metal ions for lipase stability: Structural rearrangements induced in the Burkholderia glumae lipase by calcium depletion. Journal of Structural Biology, 2009, 168, 562-570.	1.3	28
54	Dynamic Properties of a Psychrophilic Î±-Amylase in Comparison with a Mesophilic Homologue. Journal of Physical Chemistry B, 2009, 113, 13585-13595.	1.2	27

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55	Near Native-State Conformational Landscape of Psychrophilic and Mesophilic Enzymes: Probing the Folding Funnel Model. Journal of Physical Chemistry B, 2010, 114, 7609-7619.	1.2	27
56	Loop 7 of E2 Enzymes: An Ancestral Conserved Functional Motif Involved in the E2-Mediated Steps of the Ubiquitination Cascade. PLoS ONE, 2012, 7, e40786.	1.1	26
57	MutateX: an automated pipeline for in silico saturation mutagenesis of protein structures and structural ensembles. Briefings in Bioinformatics, 2022, 23, .	3.2	26
58	Intramolecular interactions stabilizing compact conformations of the intrinsically disordered kinase-inhibitor domain of Sic1: a molecular dynamics investigation. Frontiers in Physiology, 2012, 3, 435.	1.3	25
59	Structural investigation of the cold-adapted acylaminoacyl peptidase from Sporosarcina psychrophila by atomistic simulations and biophysical methods. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 2203-2213.	1.1	25
60	A single cysteine post-translational oxidation suffices to compromise globular proteins kinetic stability and promote amyloid formation. Redox Biology, 2018, 14, 566-575.	3.9	25
61	Molecular dynamics ensemble refinement of the heterogeneous native state of NCBD using chemical shifts and NOEs. PeerJ, 2018, 6, e5125.	0.9	25
62	Nâ€glycan signatures identified in tumor interstitial fluid and serum of breast cancer patients: association with tumor biology and clinical outcome. Molecular Oncology, 2018, 12, 972-990.	2.1	24
63	Structure and Dynamics in the ATG8 Family From Experimental to Computational Techniques. Frontiers in Cell and Developmental Biology, 2020, 8, 420.	1.8	24
64	A Two-step Protein Quality Control Pathway for a Misfolded DJ-1 Variant in Fission Yeast. Journal of Biological Chemistry, 2015, 290, 21141-21153.	1.6	22
65	Gaining insights into cancer biology through exploration of the cancer secretome using proteomic and bioinformatic tools. Expert Review of Proteomics, 2017, 14, 1021-1035.	1.3	21
66	Use of Computational Biochemistry for Elucidating Molecular Mechanisms of Nitric Oxide Synthase. Computational and Structural Biotechnology Journal, 2019, 17, 415-429.	1.9	21
67	The role of the central flexible region on the aggregation and conformational properties of human ataxinâ€3. FEBS Journal, 2012, 279, 451-463.	2.2	19
68	Dynamics fingerprint and inherent asymmetric flexibility of a cold-adapted homodimeric enzyme. A case study of the Vibrio alkaline phosphatase. Biochimica Et Biophysica Acta - General Subjects, 2013, 1830, 2970-2980.	1.1	19
69	Molecular and structural insight into lysine selection on substrate and ubiquitin lysine 48 by the ubiquitin-conjugating enzyme Cdc34. Cell Cycle, 2013, 12, 1732-1744.	1.3	19
70	(Dis)similarity Index To Compare Correlated Motions in Molecular Simulations. Journal of Chemical Theory and Computation, 2015, 11, 4404-4414.	2.3	19
71	The conformational and mutational landscape of the ubiquitin-like marker for autophagosome formation in cancer. Autophagy, 2021, 17, 2818-2841.	4.3	19
72	S-nitrosylation affects TRAP1 structure and ATPase activity and modulates cell response to apoptotic stimuli. Biochemical Pharmacology, 2020, 176, 113869.	2.0	19

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73	Highâ€throughput proteomics of breast cancer interstitial fluid: identification of tumor subtypeâ€specific serologically relevant biomarkers. Molecular Oncology, 2021, 15, 429-461.	2.1	19
74	A pan-cancer assessment of alterations of the kinase domain of ULK1, an upstream regulator of autophagy. Scientific Reports, 2020, 10, 14874.	1.6	18
75	C-terminal acidic domain of ubiquitin-conjugating enzymes: A multi-functional conserved intrinsically disordered domain in family 3 of E2 enzymes. Journal of Structural Biology, 2012, 178, 245-259.	1.3	17
76	A comparative study of Whi5 and retinoblastoma proteins: from sequence and structure analysis to intracellular networks. Frontiers in Physiology, 2013, 4, 315.	1.3	17
77	Flexibility of cold- and heat-adapted subtilisin-like serine proteinases evaluated with fluorescence quenching and molecular dynamics. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 705-712.	1.1	17
78	Cancer-related Mutations with Local or Long-range Effects on an Allosteric Loop of p53. Journal of Molecular Biology, 2022, 434, 167663.	2.0	17
79	Molecular dynamics investigation of cyclic natriuretic peptides: Dynamic properties reflect peptide activity. Journal of Molecular Graphics and Modelling, 2010, 28, 834-841.	1.3	16
80	Conformational Diseases: Structural Studies of Aggregation of Polyglutamine Proteins. Current Computer-Aided Drug Design, 2011, 7, 23-43.	0.8	16
81	Functional annotation of the mesophilic-like character of mutants in a cold-adapted enzyme by self-organising map analysis of their molecular dynamics. Molecular BioSystems, 2012, 8, 2680.	2.9	15
82	Molecular Dynamics Simulation of Chemokine Receptors in Lipid Bilayer: A Case Study on <scp>C</scp>â€“<scp>C</scp> Chemokine Receptor Type 2. Chemical Biology and Drug Design, 2013, 82, 534-545.	1.5	15
83	The conformational ensemble of the disordered and aggregation-protective 182â€“291 region of ataxin-3. Biochimica Et Biophysica Acta - General Subjects, 2013, 1830, 5236-5247.	1.1	14
84	Three-dimensional structure of the catalytic domain of the yeast Î²-(1,3)-glucan transferase Gas1: a molecular modeling investigation. Journal of Molecular Modeling, 2006, 12, 237-248.	0.8	13
85	eIF4A3 regulates the TFEB-mediated transcriptional response via GSK3B to control autophagy. Cell Death and Differentiation, 2021, 28, 3344-3356.	5.0	13
86	Characterization of a natural variant of human NDP52 and its functional consequences on mitophagy. Cell Death and Differentiation, 2021, 28, 2499-2516.	5.0	12
87	An intrinsically disordered proteins community for ELIXIR. F1000Research, 2019, 8, 1753.	0.8	12
88	Reciprocal Influence of Protein Domains in the Cold-Adapted Acyl Aminoacyl Peptidase from Sporosarcina psychrophila. PLoS ONE, 2013, 8, e56254.	1.1	12
89	A dual-reporter system for investigating and optimizing protein translation and folding in E. coli. Nature Communications, 2021, 12, 6093.	5.8	12
90	Zinc induced folding is essential for TIM15 activity as an mtHsp70 chaperone. Biochimica Et Biophysica Acta - General Subjects, 2013, 1830, 2139-2149.	1.1	11

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91	A single mutation Gln142Lys doubles the catalytic activity of VPR, a cold adapted subtilisin-like serine proteinase. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2016, 1864, 1436-1443.	1.1	11
92	Structural Details of BH3 Motifs and BH3-Mediated Interactions: an Updated Perspective. Frontiers in Molecular Biosciences, 2022, 9, .	1.6	11
93	Coupled motions during dynamics reveal a tunnel toward the active site regulated by the N-terminal Î±-helix in an acylaminoacyl peptidase. Journal of Molecular Graphics and Modelling, 2012, 38, 226-234.	1.3	10
94	CAncer bioMarker Prediction Pipeline (CAMPP)â€"A standardized framework for the analysis of quantitative biological data. PLoS Computational Biology, 2020, 16, e1007665.	1.5	10
95	Inhibitors of the Cdc34 acidic loop: A computational investigation integrating molecular dynamics, virtual screening and docking approaches. FEBS Open Bio, 2014, 4, 473-484.	1.0	9
96	Ion pairs and their role in modulating stability of coldâ€•and warmâ€•active uracil DNA glycosylase. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1219-1230.	1.5	8
97	Computational approaches to shed light on molecular mechanisms in biological processes. Theoretical Chemistry Accounts, 2007, 117, 723-741.	0.5	8
98	Disease-associated mutations impacting BC-loop flexibility trigger long-range transthyretin tetramer destabilization and aggregation. Journal of Biological Chemistry, 2021, 297, 101039.	1.6	8
99	Unraveling membrane properties at the organelle-level with LipidDyn. Computational and Structural Biotechnology Journal, 2022, 20, 3604-3614.	1.9	8
100	Bcl-xL Dynamics under the Lens of Protein Structure Networks. Journal of Physical Chemistry B, 2021, 125, 4308-4320.	1.2	7
101	Hybrid Voronoi diagrams, their computation and reduction for applications in computational biochemistry. Journal of Molecular Graphics and Modelling, 2017, 74, 225-233.	1.3	6
102	Ubiquitin Interacting Motifs: Duality Between Structured and Disordered Motifs. Frontiers in Molecular Biosciences, 2021, 8, 676235.	1.6	6
103	Câ€type natriuretic peptide: Structural studies, fragment synthesis, and preliminary biological evaluation in human osteosarcoma cell lines. Biopolymers, 2010, 94, 213-219.	1.2	5
104	Conformational plasticity of the calciumâ€binding pocket in the Burkholderia glumae lipase: Remodeling induced by mutation of calcium coordinating residues. Biopolymers, 2011, 95, 117-126.	1.2	4
105	Atomistic Insights Into the Regulatory Mechanisms Mediated by Post- Translational Modifications: Molecular Dynamics Investigations. Current Physical Chemistry, 2012, 2, 344-362.	0.1	4
106	Investigating Conformational Dynamics and Allostery in the p53 DNA-Binding Domain Using Molecular Simulations. Methods in Molecular Biology, 2021, 2253, 221-244.	0.4	2
107	Molecular Dynamics Simulations to Study Structure-Function Relationship in Psychrophilic Enzymes. Grand Challenges in Biology and Biotechnology, 2016, , 675-698.	2.4	1
108	Analyzing Biomolecular Ensembles. Methods in Molecular Biology, 2019, 2022, 415-451.	0.4	1

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109	Conformational gating in ammonia lyases. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129605.	1.1	1
110	Structure-function investigation of 3-methylaspartate ammonia lyase reveals substrate molecular determinants for the deamination reaction. PLoS ONE, 2020, 15, e0233467.	1.1	1
111	Atomistic Insights Into the Regulatory Mechanisms Mediated by Post- Translational Modifications: Molecular Dynamics Investigations. Current Physical Chemistry, 2012, 2, 344-362.	0.1	0
112	Title is missing!. , 2020, 16, e1007665.		0
113	Title is missing!. , 2020, 16, e1007665.		0
114	Title is missing!. , 2020, 16, e1007665.		0
115	Title is missing!. , 2020, 16, e1007665.		0
116	Title is missing!. , 2020, 16, e1007665.		0
117	Title is missing!. , 2019, 15, e1007485.		0
118	Title is missing!. , 2019, 15, e1007485.		0
119	Title is missing!. , 2019, 15, e1007485.		0