

Elena Papaleo

List of Publications by Year in descending order

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119
papers

4,707
citations

117625

34
h-index

133252

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. <i>PLoS Computational Biology</i> , 2019, 15, e1006701.	3.2	319
2	The Role of Protein Loops and Linkers in Conformational Dynamics and Allostery. <i>Chemical Reviews</i> , 2016, 116, 6391-6423.	47.7	302
3	Free-energy landscape, principal component analysis, and structural clustering to identify representative conformations from molecular dynamics simulations: The myoglobin case. <i>Journal of Molecular Graphics and Modelling</i> , 2009, 27, 889-899.	2.4	298
4	HUWE1 E3 ligase promotes PINK1/PARKIN-independent mitophagy by regulating AMBRA1 activation via IKK $\hat{\imath}$. <i>Nature Communications</i> , 2018, 9, 3755.	12.8	198
5	DisProt: intrinsic protein disorder annotation in 2020. <i>Nucleic Acids Research</i> , 2020, 48, D269-D276.	14.5	141
6	Protein aggregation: Mechanisms and functional consequences. <i>International Journal of Biochemistry and Cell Biology</i> , 2012, 44, 1541-1554.	2.8	139
7	DisProt in 2022: improved quality and accessibility of protein intrinsic disorder annotation. <i>Nucleic Acids Research</i> , 2022, 50, D480-D487.	14.5	117
8	An Efficient Method for Estimating the Hydrodynamic Radius of Disordered Protein Conformations. <i>Biophysical Journal</i> , 2017, 113, 550-557.	0.5	110
9	PyInteraph: A Framework for the Analysis of Interaction Networks in Structural Ensembles of Proteins. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1537-1551.	5.4	107
10	Predicting the impact of Lynch syndrome-causing missense mutations from structural calculations. <i>PLoS Genetics</i> , 2017, 13, e1006739.	3.5	90
11	Comparing Molecular Dynamics Force Fields in the Essential Subspace. <i>PLoS ONE</i> , 2015, 10, e0121114.	2.5	80
12	ETHE1 mutations are specific to ethylmalonic encephalopathy. <i>Journal of Medical Genetics</i> , 2005, 43, 340-346.	3.2	78
13	Flexibility and enzymatic cold-adaptation: A comparative molecular dynamics investigation of the elastase family. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2006, 1764, 1397-1406.	2.3	70
14	An optimal distance cutoff for contact-based Protein Structure Networks using side-chain centers of mass. <i>Scientific Reports</i> , 2017, 7, 2838.	3.3	70
15	Interpreting pathways to discover cancer driver genes with Moonlight. <i>Nature Communications</i> , 2020, 11, 69.	12.8	66
16	xPyder: A PyMOL Plugin To Analyze Coupled Residues and Their Networks in Protein Structures.. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1865-1874.	5.4	64
17	Integrating atomistic molecular dynamics simulations, experiments, and network analysis to study protein dynamics: strength in unity. <i>Frontiers in Molecular Biosciences</i> , 2015, 2, 28.	3.5	64
18	ENCORE: Software for Quantitative Ensemble Comparison. <i>PLoS Computational Biology</i> , 2015, 11, e1004415.	3.2	64

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19	Mapping transiently formed and sparsely populated conformations on a complex energy landscape. <i>ELife</i> , 2016, 5, .	6.0	63
20	Compaction Properties of an Intrinsically Disordered Protein: Sic1 and Its Kinase-Inhibitor Domain. <i>Biophysical Journal</i> , 2011, 100, 2243-2252.	0.5	62
21	How well do force fields capture the strength of salt bridges in proteins?. <i>PeerJ</i> , 2018, 6, e4967.	2.0	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 Ca ²⁺ . <i>Frontiers in Genetics</i> , 2015, 6, 185.	2.3	57
23	Toward mechanistic models for genotype-phenotype correlations in phenylketonuria using protein stability calculations. <i>Human Mutation</i> , 2019, 40, 444-457.	2.5	56
24	Protein flexibility in psychrophilic and mesophilic trypsins. Evidence of evolutionary conservation of protein dynamics in trypsin-like serine-proteases. <i>FEBS Letters</i> , 2008, 582, 1008-1018.	2.8	53
25	Dynamic properties of extremophilic subtilisin-like serine-proteases. <i>Journal of Structural Biology</i> , 2011, 174, 69-83.	2.8	52
26	A combined computational and structural model of the full-length human prolactin receptor. <i>Nature Communications</i> , 2016, 7, 11578.	12.8	52
27	Computational and cellular studies reveal structural destabilization and degradation of MLH1 variants in Lynch syndrome. <i>ELife</i> , 2019, 8, .	6.0	49
28	Cytokine profiling of tumor interstitial fluid of the breast and its relationship with lymphocyte infiltration and clinicopathological characteristics. <i>Oncolmmunology</i> , 2016, 5, e1248015.	4.6	48
29	Conformational Changes and Free Energies in a Proline Isomerase. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4169-4174.	5.3	46
30	The human Na ⁺ /H ⁺ exchanger 1 is a membrane scaffold protein for extracellular signal-regulated kinase 2. <i>BMC Biology</i> , 2016, 14, 31.	3.8	45
31	Molecular Determinants of Enzyme Cold Adaptation: Comparative Structural and Computational Studies of Cold- and Warm-Adapted Enzymes. <i>Current Protein and Peptide Science</i> , 2011, 12, 657-683.	1.4	44
32	E2 superfamily of ubiquitin-conjugating enzymes: constitutively active or activated through phosphorylation in the catalytic cleft. <i>Scientific Reports</i> , 2015, 5, 14849.	3.3	43
33	Alterations of the interactome of Bcl-2 proteins in breast cancer at the transcriptional, mutational and structural level. <i>PLoS Computational Biology</i> , 2019, 15, e1007485.	3.2	42
34	Mechanisms of Intramolecular Communication in a Hyperthermophilic Acylaminoacyl Peptidase: A Molecular Dynamics Investigation. <i>PLoS ONE</i> , 2012, 7, e35686.	2.5	40
35	Communication Routes in ARID Domains between Distal Residues in Helix 5 and the DNA-Binding Loops. <i>PLoS Computational Biology</i> , 2014, 10, e1003744.	3.2	40
36	DNA-binding protects p53 from interactions with cofactors involved in transcription-independent functions. <i>Nucleic Acids Research</i> , 2016, 44, gkw770.	14.5	40

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37	The role of salt bridges on the temperature adaptation of aqualysin I, a thermostable subtilisin-like proteinase. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2014, 1844, 2174-2181.	2.3	39
38	Optimization of electrostatics as a strategy for cold-adaptation: A case study of cold- and warm-active elastases. <i>Journal of Molecular Graphics and Modelling</i> , 2007, 26, 93-103.	2.4	38
39	Molecular Dynamics of Mesophilic-Like Mutants of a Cold-Adapted Enzyme: Insights into Distal Effects Induced by the Mutations. <i>PLoS ONE</i> , 2011, 6, e24214.	2.5	38
40	<i>MIR7</i> , a MYC-dependent modulator of cell proliferation, inhibits autophagy by a regulatory loop involving <i>AMBRA1</i> . <i>Autophagy</i> , 2017, 13, 554-566.	9.1	38
41	Evidence for the Formation of a Mo-H Intermediate in the Catalytic Cycle of Formate Dehydrogenase. <i>Inorganic Chemistry</i> , 2012, 51, 8331-8339.	4.0	37
42	Effects of Calcium Binding on Structure and Autolysis Regulation in Trypsins. A Molecular Dynamics Investigation. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 1286-1297.	5.3	35
43	Molecular dynamics-guided discovery of an ago-allosteric modulator for GPR40/FFAR1. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 7123-7128.	7.1	35
44	The Mutational Landscape of the Oncogenic MZF1 SCAN Domain in Cancer. <i>Frontiers in Molecular Biosciences</i> , 2016, 3, 78.	3.5	34
45	A phosphorylation-motif for tuneable helix stabilisation in intrinsically disordered proteins – Lessons from the sodium proton exchanger 1 (NHE1). <i>Cellular Signalling</i> , 2017, 37, 40-51.	3.6	34
46	Distinct signatures of lung cancer types: aberrant mucin O-glycosylation and compromised immune response. <i>BMC Cancer</i> , 2019, 19, 824.	2.6	34
47	Paths of long-range communication in the E2 enzymes of family 3: a molecular dynamics investigation. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12515.	2.8	33
48	Computational Structural Biology of S-nitrosylation of Cancer Targets. <i>Frontiers in Oncology</i> , 2018, 8, 272.	2.8	32
49	A comparative study of cold- and warm-adapted Endonucleases A using sequence analyses and molecular dynamics simulations. <i>PLoS ONE</i> , 2017, 12, e0169586.	2.5	30
50	Validation of protein models by a neural network approach. <i>BMC Bioinformatics</i> , 2008, 9, 66.	2.6	29
51	An Acidic Loop and Cognate Phosphorylation Sites Define a Molecular Switch That Modulates Ubiquitin Charging Activity in Cdc34-Like Enzymes. <i>PLoS Computational Biology</i> , 2011, 7, e1002056.	3.2	29
52	Secreted breast tumor interstitial fluid microRNAs and their target genes are associated with triple-negative breast cancer, tumor grade, and immune infiltration. <i>Breast Cancer Research</i> , 2020, 22, 73.	5.0	29
53	Relevance of metal ions for lipase stability: Structural rearrangements induced in the <i>Burkholderia glumae</i> lipase by calcium depletion. <i>Journal of Structural Biology</i> , 2009, 168, 562-570.	2.8	28
54	Dynamic Properties of a Psychrophilic α -Amylase in Comparison with a Mesophilic Homologue. <i>Journal of Physical Chemistry B</i> , 2009, 113, 13585-13595.	2.6	27

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55	Near Native-State Conformational Landscape of Psychrophilic and Mesophilic Enzymes: Probing the Folding Funnel Model. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7609-7619.	2.6	27
56	Loop 7 of E2 Enzymes: An Ancestral Conserved Functional Motif Involved in the E2-Mediated Steps of the Ubiquitination Cascade. <i>PLoS ONE</i> , 2012, 7, e40786.	2.5	26
57	MutateX: an automated pipeline for <i>in silico</i> saturation mutagenesis of protein structures and structural ensembles. <i>Briefings in Bioinformatics</i> , 2022, 23, .	6.5	26
58	Intramolecular interactions stabilizing compact conformations of the intrinsically disordered kinase-inhibitor domain of Sic1: a molecular dynamics investigation. <i>Frontiers in Physiology</i> , 2012, 3, 435.	2.8	25
59	Structural investigation of the cold-adapted acylaminoacyl peptidase from <i>Sporosarcina psychrophila</i> by atomistic simulations and biophysical methods. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2014, 1844, 2203-2213.	2.3	25
60	A single cysteine post-translational oxidation suffices to compromise globular proteins kinetic stability and promote amyloid formation. <i>Redox Biology</i> , 2018, 14, 566-575.	9.0	25
61	Molecular dynamics ensemble refinement of the heterogeneous native state of NCBD using chemical shifts and NOEs. <i>PeerJ</i> , 2018, 6, e5125.	2.0	25
62	<i>N</i> -glycan signatures identified in tumor interstitial fluid and serum of breast cancer patients: association with tumor biology and clinical outcome. <i>Molecular Oncology</i> , 2018, 12, 972-990.	4.6	24
63	Structure and Dynamics in the ATG8 Family From Experimental to Computational Techniques. <i>Frontiers in Cell and Developmental Biology</i> , 2020, 8, 420.	3.7	24
64	A Two-step Protein Quality Control Pathway for a Misfolded DJ-1 Variant in Fission Yeast. <i>Journal of Biological Chemistry</i> , 2015, 290, 21141-21153.	3.4	22
65	Gaining insights into cancer biology through exploration of the cancer secretome using proteomic and bioinformatic tools. <i>Expert Review of Proteomics</i> , 2017, 14, 1021-1035.	3.0	21
66	Use of Computational Biochemistry for Elucidating Molecular Mechanisms of Nitric Oxide Synthase. <i>Computational and Structural Biotechnology Journal</i> , 2019, 17, 415-429.	4.1	21
67	The role of the central flexible region on the aggregation and conformational properties of human ataxin-3. <i>FEBS Journal</i> , 2012, 279, 451-463.	4.7	19
68	Dynamics fingerprint and inherent asymmetric flexibility of a cold-adapted homodimeric enzyme. A case study of the <i>Vibrio</i> alkaline phosphatase. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2013, 1830, 2970-2980.	2.4	19
69	Molecular and structural insight into lysine selection on substrate and ubiquitin lysine 48 by the ubiquitin-conjugating enzyme Cdc34. <i>Cell Cycle</i> , 2013, 12, 1732-1744.	2.6	19
70	(Dis)similarity Index To Compare Correlated Motions in Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4404-4414.	5.3	19
71	The conformational and mutational landscape of the ubiquitin-like marker for autophagosome formation in cancer. <i>Autophagy</i> , 2021, 17, 2818-2841.	9.1	19
72	S-nitrosylation affects TRAP1 structure and ATPase activity and modulates cell response to apoptotic stimuli. <i>Biochemical Pharmacology</i> , 2020, 176, 113869.	4.4	19

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73	High-throughput proteomics of breast cancer interstitial fluid: identification of tumor subtype-specific serologically relevant biomarkers. <i>Molecular Oncology</i> , 2021, 15, 429-461.	4.6	19
74	A pan-cancer assessment of alterations of the kinase domain of ULK1, an upstream regulator of autophagy. <i>Scientific Reports</i> , 2020, 10, 14874.	3.3	18
75	C-terminal acidic domain of ubiquitin-conjugating enzymes: A multi-functional conserved intrinsically disordered domain in family 3 of E2 enzymes. <i>Journal of Structural Biology</i> , 2012, 178, 245-259.	2.8	17
76	A comparative study of Whi5 and retinoblastoma proteins: from sequence and structure analysis to intracellular networks. <i>Frontiers in Physiology</i> , 2013, 4, 315.	2.8	17
77	Flexibility of cold- and heat-adapted subtilisin-like serine proteinases evaluated with fluorescence quenching and molecular dynamics. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2014, 1844, 705-712.	2.3	17
78	Cancer-related Mutations with Local or Long-range Effects on an Allosteric Loop of p53. <i>Journal of Molecular Biology</i> , 2022, 434, 167663.	4.2	17
79	Molecular dynamics investigation of cyclic natriuretic peptides: Dynamic properties reflect peptide activity. <i>Journal of Molecular Graphics and Modelling</i> , 2010, 28, 834-841.	2.4	16
80	Conformational Diseases: Structural Studies of Aggregation of Polyglutamine Proteins. <i>Current Computer-Aided Drug Design</i> , 2011, 7, 23-43.	1.2	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. <i>Molecular BioSystems</i> , 2012, 8, 2680.	2.9	15
82	Molecular Dynamics Simulation of Chemokine Receptors in Lipid Bilayer: A Case Study on Chemokine Receptor Type 2. <i>Chemical Biology and Drug Design</i> , 2013, 82, 534-545.	3.2	15
83	The conformational ensemble of the disordered and aggregation-protective 182-291 region of ataxin-3. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2013, 1830, 5236-5247.	2.4	14
84	Three-dimensional structure of the catalytic domain of the yeast β -(1,3)-glucan transferase Gas1: a molecular modeling investigation. <i>Journal of Molecular Modeling</i> , 2006, 12, 237-248.	1.8	13
85	eIF4A3 regulates the TFEB-mediated transcriptional response via GSK3B to control autophagy. <i>Cell Death and Differentiation</i> , 2021, 28, 3344-3356.	11.2	13
86	Characterization of a natural variant of human NDP52 and its functional consequences on mitophagy. <i>Cell Death and Differentiation</i> , 2021, 28, 2499-2516.	11.2	12
87	An intrinsically disordered proteins community for ELIXIR. <i>F1000Research</i> , 2019, 8, 1753.	1.6	12
88	Reciprocal Influence of Protein Domains in the Cold-Adapted Acyl Aminoacyl Peptidase from <i>Sporosarcina psychrophila</i> . <i>PLoS ONE</i> , 2013, 8, e56254.	2.5	12
89	A dual-reporter system for investigating and optimizing protein translation and folding in <i>E. coli</i> . <i>Nature Communications</i> , 2021, 12, 6093.	12.8	12
90	Zinc induced folding is essential for TIM15 activity as an mtHsp70 chaperone. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2013, 1830, 2139-2149.	2.4	11

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91	A single mutation Gln142Lys doubles the catalytic activity of VPR, a cold adapted subtilisin-like serine proteinase. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2016, 1864, 1436-1443.	2.3	11
92	Structural Details of BH3 Motifs and BH3-Mediated Interactions: an Updated Perspective. <i>Frontiers in Molecular Biosciences</i> , 2022, 9, .	3.5	11
93	Coupled motions during dynamics reveal a tunnel toward the active site regulated by the N-terminal α -helix in an acylaminoacyl peptidase. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 38, 226-234.	2.4	10
94	CANcer bioMarker Prediction Pipeline (CAMPP)â€”A standardized framework for the analysis of quantitative biological data. <i>PLoS Computational Biology</i> , 2020, 16, e1007665.	3.2	10
95	Inhibitors of the Cdc34 acidic loop: A computational investigation integrating molecular dynamics, virtual screening and docking approaches. <i>FEBS Open Bio</i> , 2014, 4, 473-484.	2.3	9
96	Ion pairs and their role in modulating stability of coldâ€”and warmâ€”active uracil DNA glycosylase. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 71, 1219-1230.	2.6	8
97	Computational approaches to shed light on molecular mechanisms in biological processes. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 723-741.	1.4	8
98	Disease-associated mutations impacting BC-loop flexibility trigger long-range transthyretin tetramer destabilization and aggregation. <i>Journal of Biological Chemistry</i> , 2021, 297, 101039.	3.4	8
99	Unraveling membrane properties at the organelle-level with LipidDyn. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 3604-3614.	4.1	8
100	Bcl-xL Dynamics under the Lens of Protein Structure Networks. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4308-4320.	2.6	7
101	Hybrid Voronoi diagrams, their computation and reduction for applications in computational biochemistry. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 74, 225-233.	2.4	6
102	Ubiquitin Interacting Motifs: Duality Between Structured and Disordered Motifs. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 676235.	3.5	6
103	Câ€”type natriuretic peptide: Structural studies, fragment synthesis, and preliminary biological evaluation in human osteosarcoma cell lines. <i>Biopolymers</i> , 2010, 94, 213-219.	2.4	5
104	Conformational plasticity of the calciumâ€”binding pocket in the <i>Burkholderia glumae</i> lipase: Remodeling induced by mutation of calcium coordinating residues. <i>Biopolymers</i> , 2011, 95, 117-126.	2.4	4
105	Atomistic Insights Into the Regulatory Mechanisms Mediated by Post- Translational Modifications: Molecular Dynamics Investigations. <i>Current Physical Chemistry</i> , 2012, 2, 344-362.	0.2	4
106	Investigating Conformational Dynamics and Allostery in the p53 DNA-Binding Domain Using Molecular Simulations. <i>Methods in Molecular Biology</i> , 2021, 2253, 221-244.	0.9	2
107	Molecular Dynamics Simulations to Study Structure-Function Relationship in Psychrophilic Enzymes. <i>Grand Challenges in Biology and Biotechnology</i> , 2016, , 675-698.	2.4	1
108	Analyzing Biomolecular Ensembles. <i>Methods in Molecular Biology</i> , 2019, 2022, 415-451.	0.9	1

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109	Conformational gating in ammonia lyases. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2020, 1864, 129605.	2.4	1
110	Structure-function investigation of 3-methylaspartate ammonia lyase reveals substrate molecular determinants for the deamination reaction. <i>PLoS ONE</i> , 2020, 15, e0233467.	2.5	1
111	Atomistic Insights Into the Regulatory Mechanisms Mediated by Post- Translational Modifications: Molecular Dynamics Investigations. <i>Current Physical Chemistry</i> , 2012, 2, 344-362.	0.2	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