Panagiotis L Kastritis

List of Publications by Year
in descending order

64 papers	6,967 citations	147566 31 h-index	114278 63 g-index
75 all docs	75 docs citations	75 times ranked	9919 citing authors

#	Article	IF	Citations
1	The HADDOCK2.2 Web Server: User-Friendly Integrative Modeling of Biomolecular Complexes. Journal of Molecular Biology, 2016, 428, 720-725.	2.0	2,071
2	PRODIGY: a web server for predicting the binding affinity of proteinâ€“protein complexes. Bioinformatics, 2016, 32, 3676-3678.	1.8	760
3	In situ structural analysis of the human nuclear pore complex. Nature, 2015, 526, 140-143.	13.7	361
4	On the binding affinity of macromolecular interactions: daring to ask why proteins interact. Journal of the Royal Society Interface, 2013, 10, 20120835.	1.5	353
5	Updates to the Integrated Proteinâ€“Protein Interaction Benchmarks: Docking Benchmark Version 5 and Affinity Benchmark Version 2. Journal of Molecular Biology, 2015, 427, 3031-3041.	2.0	348
6	A structureâ€based benchmark for proteinâ€“protein binding affinity. Protein Science, 2011, 20, 482-491.	3.1	252
7	Are Scoring Functions in Proteinâ€'Protein Docking Ready To Predict Interactomes? Clues from a Novel Binding Affinity Benchmark. Journal of Proteome Research, 2010, 9, 2216-2225.	1.8	224
8	Structure and Assembly of the Nuclear Pore Complex. Annual Review of Biophysics, 2019, 48, 515-536.	4.5	205
9	Prediction of homoprotein and heteroprotein complexes by protein docking and templateâ€based modeling: A CASPâ€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2016, 84, 323-348.	1.5	148
10	Antimicrobial and Efflux Pump Inhibitory Activity of Caffeoylquinic Acids from Artemisia absinthium against Gram-Positive Pathogenic Bacteria. PLoS ONE, 2011, 6, e18127.	1.1	133
11	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302.	2.0	131
12	Spatiotemporal variation of mammalian protein complex stoichiometries. Genome Biology, 2016, 17, 47.	3.8	115
13	Building Macromolecular Assemblies by Information-driven Docking. Molecular and Cellular Proteomics, 2010, 9, 1784-1794.	2.5	114
14	Capturing protein communities by structural proteomics in a thermophilic eukaryote. Molecular Systems Biology, 2017, 13, 936.	3.2	108
15	Clustering biomolecular complexes by residue contacts similarity. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1810-1817.	1.5	103
16	Proteins Feel More Than They See: Fine-Tuning of Binding Affinity by Properties of the Non-Interacting Surface. Journal of Molecular Biology, 2014, 426, 2632-2652.	2.0	103
17	Cross-Linking Mass Spectrometry for Investigating Protein Conformations and Proteinâ€“Protein Interactionsâ€”A Method for All Seasons. Chemical Reviews, 2022, 122, 7500-7531.	23.0	101
18	Subnanometre-resolution structure of the doublet microtubule reveals new classes of microtubule-associated proteins. Nature Communications, 2017, 8, 15035.	5.8	98

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19	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1980-1987.	1.5	87
20	dMM-PBSA: A New HADDOCK Scoring Function for Protein-Peptide Docking. Frontiers in Molecular Biosciences, 2016, 3, 46.	1.6	67
21	Structural basis for assembly and function of the Nup82 complex in the nuclear pore scaffold. Journal of Cell Biology, 2015, 208, 283-297.	2.3	64
22	Defining the limits of homology modeling in informationâ€driven protein docking. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2119-2128.	1.5	63
23	Haloadaptation: Insights from comparative modeling studies of halophilic archaeal DHFRs. International Journal of Biological Macromolecules, 2007, 41, 447-453.	3.6	58
24	An integrated approach for genome annotation of the eukaryotic thermophile Chaetomium thermophilum. Nucleic Acids Research, 2014, 42, 13525-13533.	6.5	55
25	Insights on cross-species transmission of SARS-CoV-2 from structural modeling. PLoS Computational Biology, 2020, 16, e1008449.	1.5	52
26	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	1.5	50
27	Sense and simplicity in <scp>HADDOCK</scp> scoring: Lessons from <scp>CASPâ€CAPRI</scp> round 1. Proteins: Structure, Function and Bioinformatics, 2017, 85, 417-423.	1.5	44
28	Enzymatic complexes across scales. Essays in Biochemistry, 2018, 62, 501-514.	2.1	40
29	Flexibility of intrinsically disordered degrons in AUX/IAA proteins reinforces auxin co-receptor assemblies. Nature Communications, 2020, 11, 2277.	5.8	38
30	Molecular origins of binding affinity: seeking the Archimedean point. Current Opinion in Structural Biology, 2013, 23, 868-877.	2.6	37
31	Constructing artificial respiratory chain in polymer compartments: Insights into the interplay betweenbo₃oxidase and the membrane. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 15006-15017.	3.3	37
32	Strengths and weaknesses of dataâ€driven docking in critical assessment of prediction of interactions. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3242-3249.	1.5	36
33	Integrative structure of a 10-megadalton eukaryotic pyruvate dehydrogenase complex from native cell extracts. Cell Reports, 2021, 34, 108727.	2.9	36
34	Cryo-EM and artificial intelligence visualize endogenous protein community members. Structure, 2022, 30, 575-589.e6.	1.6	31
35	HADDOCK_{2P2I}: A Biophysical Model for Predicting the Binding Affinity of Proteinâ€“Protein Interaction Inhibitors. Journal of Chemical Information and Modeling, 2014, 54, 826-836.	2.5	30
36	Structural analysis of 70S ribosomes by cross-linking/mass spectrometry reveals conformational plasticity. Scientific Reports, 2020, 10, 12618.	1.6	27

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37	Next challenges in proteinâ€“protein docking: from proteome to interactome and beyond. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 642-651.	6.2	26
38	Solvated proteinâ€“protein docking using Kyteâ€Doolittleâ€based water preferences. Proteins: Structure, Function and Bioinformatics, 2013, 81, 510-518.	1.5	26
39	Structural models of human ACE2 variants with SARS-CoV-2 Spike protein for structure-based drug design. Scientific Data, 2020, 7, 309.	2.4	26
40	Cryo-EM snapshots of a native lysate provide structural insights into a metabolon-embedded transacetylase reaction. Nature Communications, 2021, 12, 6933.	5.8	26
41	Solvated proteinâ€“DNA docking using HADDOCK. Journal of Biomolecular NMR, 2013, 56, 51-63.	1.6	23
42	Non-interacting surface solvation and dynamics in protein-protein interactions. Proteins: Structure, Function and Bioinformatics, 2015, 83, 445-458.	1.5	22
43	Integrative biology of native cell extracts: a new era for structural characterization of life processes. Biological Chemistry, 2019, 400, 831-846.	1.2	21
44	Structural impact of K63 ubiquitin on yeast translocating ribosomes under oxidative stress. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 22157-22166.	3.3	21
45	En route to dynamic life processes by SNARE-mediated fusion of polymer and hybrid membranes. Nature Communications, 2021, 12, 4972.	5.8	21
46	Explicit Treatment of Water Molecules in Data-Driven Proteinâ€“Protein Docking: The Solvated HADDOCKing Approach. Methods in Molecular Biology, 2012, 819, 355-374.	0.4	20
47	Defining distance restraints in HADDOCK. Nature Protocols, 2018, 13, 1503-1503.	5.5	18
48	Unstructured regions of large enzymatic complexes control the availability of metabolites with signaling functions. Cell Communication and Signaling, 2020, 18, 136.	2.7	14
49	The Combination of X-Ray Crystallography and Cryo-Electron Microscopy Provides Insight into the Overall Architecture of the Dodecameric Rvb1/Rvb2 Complex. PLoS ONE, 2016, 11, e0146457.	1.1	14
50	Cryo-EM structure of a tetrameric photosystem I from Chroococcidiopsis TS-821, a thermophilic, unicellular, non-heterocyst-forming cyanobacterium. Plant Communications, 2022, 3, 100248.	3.6	14
51	Increased efficiency of charge-mediated fusion in polymer/lipid hybrid membranes. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2122468119.	3.3	13
52	Detecting Protein Communities in Native Cell Extracts by Machine Learning: A Structural Biologistâ€™s Perspective. Frontiers in Molecular Biosciences, 2021, 8, 660542.	1.6	10
53	Solubilization of artificial mitochondrial membranes by amphiphilic copolymers of different charge. Biochimica Et Biophysica Acta - Biomembranes, 2021, 1863, 183725.	1.4	10
54	2.7 Ã… cryo-EM structure of vitrified M. musculus H-chain apoferritin from a compact 200 keV cryo-microscope. PLoS ONE, 2020, 15, e0232540.	1.1	9

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55	Enhanced optical imaging properties of lipid nanocapsules as vehicles for fluorescent conjugated polymers. European Journal of Pharmaceutics and Biopharmaceutics, 2020, 154, 297-308.	2.0	8
56	New potential peptide therapeutics perturbing CK1Î´/Î±-tubulin interaction. Cancer Letters, 2016, 375, 375-383.	3.2	7
57	Coupling proteomics and metabolomics for the unsupervised identification of proteinâ€“metabolite interactions in Chaetomium thermophilum. PLoS ONE, 2021, 16, e0254429.	1.1	5
58	BRCA1-BRCT Mutations Alter the Subcellular Localization of BRCA1 In Vitro. Anticancer Research, 2021, 41, 2953-2962.	0.5	4
59	First 3D-Structural Data of Full-Length Guanylyl Cyclase 1 in Rod-Outer-Segment Preparations of Bovine Retina by Cross-Linking/Mass Spectrometry. Journal of Molecular Biology, 2021, 433, 166947.	2.0	3
60	Nanoscale Model System for the Human Myelin Sheath. Biomacromolecules, 2021, 22, 3901-3912.	2.6	3
61	Thinâ€Layer Chromatography and Coomassie Staining of Phospholipids for Fast and Simple Lipidomics Sample Preparation. Analysis & Sensing, 2021, 1, 171-179.	1.1	2
62	Filling the Gap with Long n-Alkanes: Incorporation of C20 and C30 into Phospholipid Membranes. Langmuir, 2022, 38, 8595-8606.	1.6	2
63	An Electrostatically-steered Conformational Selection Mechanism Promotes SARS-CoV-2 Spike Protein Variation. Journal of Molecular Biology, 2022, 434, 167637.	2.0	1
64	Thinâ€Layer Chromatography and Coomassie Staining of Phospholipids for Fast and Simple Lipidomics Sample Preparation. Analysis & Sensing, 2021, 1, 134.	1.1	0