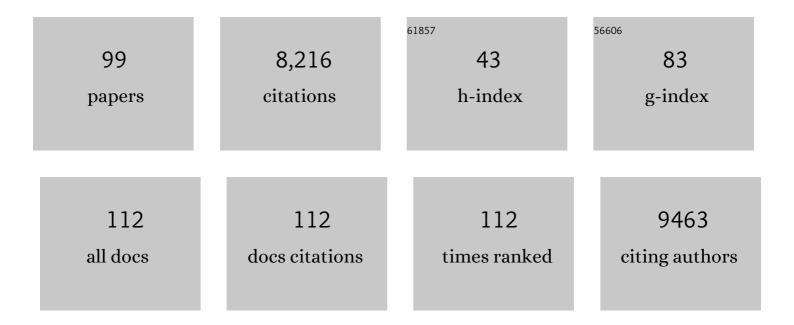
List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/3172957/publications.pdf Version: 2024-02-01



#	Article	IF	CITATIONS
1	Protein–Protein Docking with Simultaneous Optimization of Rigid-body Displacement and Side-chain Conformations. Journal of Molecular Biology, 2003, 331, 281-299.	2.0	1,017
2	Harnessing protein folding neural networks for peptide–protein docking. Nature Communications, 2022, 13, 176.	5.8	682
3	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	9.0	513
4	Sub-angstrom modeling of complexes between flexible peptides and globular proteins. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2029-2040.	1.5	384
5	The Structural Basis of Peptide-Protein Binding Strategies. Structure, 2010, 18, 188-199.	1.6	370
6	Rosetta FlexPepDock web server—high resolution modeling of peptide–protein interactions. Nucleic Acids Research, 2011, 39, W249-W253.	6.5	351
7	Progress in Modeling of Protein Structures and Interactions. Science, 2005, 310, 638-642.	6.0	271
8	Rosetta FlexPepDock ab-initio: Simultaneous Folding, Docking and Refinement of Peptides onto Their Receptors. PLoS ONE, 2011, 6, e18934.	1.1	259
9	Improved side-chain modeling for protein-protein docking. Protein Science, 2005, 14, 1328-1339.	3.1	215
10	Protein–peptide docking: opportunities and challenges. Drug Discovery Today, 2018, 23, 1530-1537.	3.2	212
11	Druggable protein–protein interactions – from hot spots to hot segments. Current Opinion in Chemical Biology, 2013, 17, 952-959.	2.8	199
12	Rosetta predictions in CASP5: Successes, failures, and prospects for complete automation. Proteins: Structure, Function and Bioinformatics, 2003, 53, 457-468.	1.5	162
13	Application of asymmetric statistical potentials to antibody–protein docking. Bioinformatics, 2012, 28, 2608-2614.	1.8	156
14	Structureâ€based prediction of binding peptides to MHC class I molecules: Application to a broad range of MHC alleles. Protein Science, 2000, 9, 1838-1846.	3.1	149
15	Can selfâ€inhibitory peptides be derived from the interfaces of globular protein–protein interactions?. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3140-3149.	1.5	146
16	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302.	2.0	131
17	Relacin, a Novel Antibacterial Agent Targeting the Stringent Response. PLoS Pathogens, 2012, 8, e1002925.	2.1	130
18	High-resolution global peptide-protein docking using fragments-based PIPER-FlexPepDock. PLoS Computational Biology, 2017, 13, e1005905.	1.5	119

#	Article	IF	CITATIONS
19	Ubiquitination and Degradation of the Inhibitors of NF-ÂB. Cold Spring Harbor Perspectives in Biology, 2010, 2, a000166-a000166.	2.3	108
20	Protein-protein docking predictions for the CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2003, 52, 118-122.	1.5	102
21	ClusPro PeptiDock: efficient global docking of peptide recognition motifs using FFT. Bioinformatics, 2017, 33, 3299-3301.	1.8	102
22	Detection of peptideâ€binding sites on protein surfaces: The first step toward the modeling and targeting of peptideâ€mediated interactions. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2096-2105.	1.5	95
23	Progress in protein-protein docking: Atomic resolution predictions in the CAPRI experiment using RosettaDock with an improved treatment of side-chain flexibility. Proteins: Structure, Function and Bioinformatics, 2005, 60, 187-194.	1.5	92
24	Folding of the C-terminal bacterial binding domain in statherin upon adsorption onto hydroxyapatite crystals. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 16083-16088.	3.3	88
25	Fractured genes: a novel genomic arrangement involving new split inteins and a new homing endonuclease family. Nucleic Acids Research, 2009, 37, 2560-2573.	6.5	86
26	The Escherichia coli Extracellular Death Factor EDF Induces the Endoribonucleolytic Activities of the Toxins MazF and ChpBK. Molecular Cell, 2011, 41, 625-635.	4.5	86
27	Peptide docking and structure-based characterization of peptide binding: from knowledge to know-how. Current Opinion in Structural Biology, 2013, 23, 894-902.	2.6	85
28	Learning MHC I–peptide binding. Bioinformatics, 2006, 22, e227-e235.	1.8	83
29	Mitochondrial complex IV deficiency, caused by mutated COX6B1, is associated with encephalomyopathy, hydrocephalus and cardiomyopathy. European Journal of Human Genetics, 2015, 23, 159-164.	1.4	82
30	Peptiderive server: derive peptide inhibitors from protein–protein interactions. Nucleic Acids Research, 2016, 44, W536-W541.	6.5	77
31	Pleiotropic Functions of Tumor Suppressor WWOX in Normal and Cancer Cells. Journal of Biological Chemistry, 2015, 290, 30728-30735.	1.6	64
32	Computational approaches to investigating allostery. Current Opinion in Structural Biology, 2016, 41, 159-171.	2.6	63
33	Conserved residue clustering and protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2003, 52, 225-235.	1.5	61
34	Encounter complexes and dimensionality reduction in protein–protein association. ELife, 2014, 3, e01370.	2.8	61
35	Rapid Sampling of Molecular Motions with Prior Information Constraints. PLoS Computational Biology, 2009, 5, e1000295.	1.5	58
36	Identification of a Novel Class of Farnesylation Targets by Structure-Based Modeling of Binding Specificity. PLoS Computational Biology, 2011, 7, e1002170.	1.5	58

#	Article	IF	CITATIONS
37	A model of anthrax toxin lethal factor bound to protective antigen. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 16409-16414.	3.3	55
38	Pathogens Use Structural Mimicry of Native Host Ligands as a Mechanism for Host Receptor Engagement. Cell Host and Microbe, 2013, 14, 63-73.	5.1	54
39	Myelin-associated glycoprotein gene mutation causes Pelizaeus-Merzbacher disease-like disorder. Brain, 2015, 138, 2521-2536.	3.7	50
40	Is GAS1 a co-receptor for the GDNF family of ligands?. Trends in Pharmacological Sciences, 2006, 27, 72-77.	4.0	49
41	Trans Protein Splicing of Cyanobacterial Split Inteins in Endogenous and Exogenous Combinations. Biochemistry, 2007, 46, 322-330.	1.2	49
42	Knowledge-based structure prediction of MHC class I bound peptides: a study of 23 complexes. Folding & Design, 1998, 3, 549-564.	4.5	47
43	Minimizing and Learning Energy Functions for Side-Chain Prediction. Journal of Computational Biology, 2008, 15, 899-911.	0.8	45
44	The structure, dynamics, and energetics of protein adsorption—lessons learned from adsorption of statherin to hydroxyapatite. Magnetic Resonance in Chemistry, 2007, 45, S32-S47.	1.1	44
45	Structure-Based Identification of HDAC8 Non-histone Substrates. Structure, 2016, 24, 458-468.	1.6	42
46	Discrimination of nearâ€native structures in protein–protein docking by testing the stability of local minima. Proteins: Structure, Function and Bioinformatics, 2008, 72, 993-1004.	1.5	41
47	<i>In Silico</i> and <i>in Vitro</i> Elucidation of BH3 Binding Specificity toward Bcl-2. Biochemistry, 2012, 51, 5841-5850.	1.2	35
48	Versatile communication strategies among tandem WW domain repeats. Experimental Biology and Medicine, 2015, 240, 351-360.	1.1	32
49	Modeling Peptide-Protein Structure and Binding Using Monte Carlo Sampling Approaches: Rosetta FlexPepDock and FlexPepBind. Methods in Molecular Biology, 2017, 1561, 139-169.	0.4	32
50	Anchoring of bacterial effectors to host membranes through host-mediated lipidation by prenylation: a common paradigm. Trends in Microbiology, 2011, 19, 573-579.	3.5	31
51	Funnel Hunting in a Rough Terrain: Learning and Discriminating Native Energy Funnels. Structure, 2008, 16, 269-279.	1.6	30
52	A benchmark testing ground for integrating homology modeling and protein docking. Proteins: Structure, Function and Bioinformatics, 2017, 85, 10-16.	1.5	29
53	Better together: Elements of successful scientific software development in a distributed collaborative community. PLoS Computational Biology, 2020, 16, e1007507.	1.5	27
54	Identifying a common molecular mechanism for inhibition of MITF and STAT3 by PIAS3. Blood, 2006, 107, 2839-2845.	0.6	26

#	Article	IF	CITATIONS
55	RosettaDock in CAPRI rounds 6–12. Proteins: Structure, Function and Bioinformatics, 2007, 69, 758-763.	1.5	26
56	Modeling Peptide–Protein Interactions. Methods in Molecular Biology, 2011, 857, 375-398.	0.4	26
57	<i><scp>MYORG</scp></i> is associated with recessive primary familial brain calcification. Annals of Clinical and Translational Neurology, 2019, 6, 106-113.	1.7	25
58	c-Abl Phosphorylates E6AP and Regulates Its E3 Ubiquitin Ligase Activity. Biochemistry, 2013, 52, 3119-3129.	1.2	23
59	Parkin Somatic Mutations Link Melanoma and Parkinson's Disease. Journal of Genetics and Genomics, 2016, 43, 369-379.	1.7	23
60	Autophosphorylation Activates Dictyostelium Myosin II Heavy Chain Kinase A by Providing a Ligand for an Allosteric Binding Site in the α-Kinase Domain. Journal of Biological Chemistry, 2011, 286, 2607-2616.	1.6	22
61	Extending RosettaDock with water, sugar, and pH for prediction of complex structures and affinities for CAPRI rounds 20–27. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2201-2209.	1.5	22
62	Structural basis for UFM1 transfer from UBA5 to UFC1. Nature Communications, 2021, 12, 5708.	5.8	21
63	FlexPepDock lessons from CAPRI peptide–protein rounds and suggested new criteria for assessment of model quality and utility. Proteins: Structure, Function and Bioinformatics, 2017, 85, 445-462.	1.5	19
64	CladeOScope: functional interactions through the prism of clade-wise co-evolution. NAR Genomics and Bioinformatics, 2021, 3, lqab024.	1.5	19
65	Molecular pathogenesis of human CD59 deficiency. Neurology: Genetics, 2018, 4, e280.	0.9	17
66	Examination of possible structural constraints of MHC-binding peptides by assessment of their native structure within their source proteins. Proteins: Structure, Function and Bioinformatics, 2001, 45, 47-54.	1.5	16
67	FunHunt: model selection based on energy landscape characteristics. Biochemical Society Transactions, 2008, 36, 1418-1421.	1.6	16
68	The SV40 Capsid Is Stabilized by a Conserved Pentapeptide Hinge of the Major Capsid Protein VP1. Journal of Molecular Biology, 2009, 386, 1382-1391.	2.0	16
69	Indirect ELISAâ€based approach for comparative measurement of highâ€affinity cohesin–dockerin interactions. Journal of Molecular Recognition, 2012, 25, 616-622.	1.1	16
70	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Nature Communications, 2021, 12, 6947.	5.8	16
71	Matching protein surface structural patches for high-resolution blind peptide docking. Proceedings of the United States of America, 2022, 119, e2121153119.	3.3	16
72	Assessing the energy landscape of CAPRI targets by FunHunt. Proteins: Structure, Function and Bioinformatics, 2007, 69, 809-815.	1.5	15

#	Article	IF	CITATIONS
73	Rationally designed macrocyclic peptides as synergistic agonists ofÂLPS-induced inflammatory response. Tetrahedron, 2014, 70, 7664-7668.	1.0	15
74	Evolving Dual Targeting of a Prokaryotic Protein in Yeast. Molecular Biology and Evolution, 2013, 30, 1563-1573.	3.5	14
75	Crucial Roles of Single Residues in Binding Affinity, Specificity, and Promiscuity in the Cellulosomal Cohesin-Dockerin Interface. Journal of Biological Chemistry, 2015, 290, 13654-13666.	1.6	14
76	Novel Structural Mechanism of Allosteric Regulation of Aspartic Peptidases via an Evolutionarily Conserved Exosite. Cell Chemical Biology, 2018, 25, 318-329.e4.	2.5	14
77	Escherichia coli Quorum-Sensing EDF, A Peptide Generated by Novel Multiple Distinct Mechanisms and Regulated by <i>trans</i> -Translation. MBio, 2016, 7, e02034-15.	1.8	13
78	Host FIH-Mediated Asparaginyl Hydroxylation of Translocated Legionella pneumophila Effectors. Frontiers in Cellular and Infection Microbiology, 2017, 7, 54.	1.8	11
79	On the use of structural templates for highâ€resolution docking. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1939-1949.	1.5	10
80	Yeast aconitase mitochondrial import is modulated by interactions of its C and N terminal domains and Ssa1/2 (Hsp70). Scientific Reports, 2018, 8, 5903.	1.6	10
81	Modeling betaâ€sheet peptideâ€protein interactions: Rosetta FlexPepDock in CAPRI rounds 38â€45. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1037-1049.	1.5	10
82	Increased sequence conservation of domain repeats in prokaryotic proteins. Trends in Genetics, 2010, 26, 383-387.	2.9	8
83	Detection of Peptide-Binding Sites on Protein Surfaces Using the Peptimap Server. Methods in Molecular Biology, 2017, 1561, 11-20.	0.4	8
84	Protocols for All-Atom Reconstruction and High-Resolution Refinement of Protein–Peptide Complex Structures. Methods in Molecular Biology, 2020, 2165, 273-287.	0.4	7
85	Structure-based prediction of HDAC6 substrates validated by enzymatic assay reveals determinants of promiscuity and detects new potential substrates. Scientific Reports, 2022, 12, 1788.	1.6	7
86	Measurements of Relative Binding of Cohesin and Dockerin Mutants Using an Advanced ELISA Technique for High-Affinity Interactions. Methods in Enzymology, 2012, 510, 417-428.	0.4	6
87	Phosphorylation of the WWOX Protein Regulates Its Interaction with p73. ChemBioChem, 2020, 21, 1843-1851.	1.3	6
88	ClusPro in rounds 38 to 45 of CAPRI: Toward combining templateâ€based methods with free docking. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1082-1090.	1.5	5
89	A unique -associated variant in a Georgian Jewish family with probable North Carolina macular dystrophy and the possible contribution of a unique variant. Molecular Vision, 2020, 26, 299-310.	1.1	5
90	Identification of autosomal recessive novel genes and retinal phenotypes in members of the solute carrier (SLC) superfamily. Genetics in Medicine, 2022, 24, 1523-1535.	1.1	5

#	Article	IF	CITATIONS
91	Minimizing and Learning Energy Functions for Side-Chain Prediction. , 2007, , 381-395.		4
92	Structural insights into the role of the WW2 domain on tandem WW–PPxY motif interactions of oxidoreductase WWOX. Journal of Biological Chemistry, 2022, 298, 102145.	1.6	4
93	A Versatile Synthetic Affinity Probe Reveals Inhibitory Synapse Ultrastructure and Brain Connectivity. Angewandte Chemie - International Edition, 2022, , .	7.2	3
94	Targeting an Interaction Between Two Disordered Domains by Using a Designed Peptide. Chemistry - A European Journal, 2020, 26, 10156-10156.	1.7	2
95	Targeting an Interaction Between Two Disordered Domains by Using a Designed Peptide. Chemistry - A European Journal, 2020, 26, 10240-10249.	1.7	2
96	Multi-system neurological disorder associated with a CRYAB variant. Neurogenetics, 2021, 22, 117-125.	0.7	1
97	High-resolution Protein–Protein Docking. , 2010, , 209-235.		0
98	Structure-Based Characterization of Peptide-Mediated Protein Interactions. Biophysical Journal, 2012, 102, 439a.	0.2	0
99	A Versatile Synthetic Affinity Probe Reveals Inhibitory Synapse Ultrastructure and Brain Connectivity. Angewandte Chemie, 0, , .	1.6	Ο