Ruth Nussinov

List of Publications by Year
in descending order

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314 papers	31,524 citations	6592 79 h-index	5806 161 g-index
323 all docs	323 docs citations	323 times ranked	27287 citing authors

#	Article	IF	Citations
1	PatchDock and SymmDock: servers for rigid and symmetric docking. Nucleic Acids Research, 2005, 33, W363-W367.	6.5	2,610
2	The role of dynamic conformational ensembles in biomolecular recognition. Nature Chemical Biology, 2009, 5, 789-796.	3.9	1,649
3	Shape complementarity at protein-protein interfaces. Biopolymers, 1994, 34, 933-940.	1.2	991
4	Is allostery an intrinsic property of all dynamic proteins?. Proteins: Structure, Function and Bioinformatics, 2004, 57, 433-443.	1.5	779
5	Structure and dynamics of molecular networks: A novel paradigm of drug discovery. , 2013, 138, 333-408.		779
6	Induced fit, conformational selection and independent dynamic segments: an extended view of binding events. Trends in Biochemical Sciences, 2010, 35, 539-546.	3.7	708
7	AÎ²(1â€“42) fibril structure illuminates self-recognition and replication of amyloid in Alzheimer's disease. Nature Structural and Molecular Biology, 2015, 22, 499-505.	3.6	701
8	FireDock: a web server for fast interaction refinement in molecular docking. Nucleic Acids Research, 2008, 36, W229-W232.	6.5	657
9	Folding funnels, binding funnels, and protein function. Protein Science, 1999, 8, 1181-1190.	3.1	634
10	FireDock: Fast interaction refinement in molecular docking. Proteins: Structure, Function and Bioinformatics, 2007, 69, 139-159.	1.5	607
11	Allostery in Disease and in Drug Discovery. Cell, 2013, 153, 293-305.	13.5	586
12	Principles of Proteinâ'Protein Interactions: What are the Preferred Ways For Proteins To Interact?. Chemical Reviews, 2008, 108, 1225-1244.	23.0	568
13	Folding funnels and binding mechanisms. Protein Engineering, Design and Selection, 1999, 12, 713-720.	1.0	534
14	Folding and binding cascades: Dynamic landscapes and population shifts. Protein Science, 2000, 9, 10-19.	3.1	521
15	Hot Regions in Proteinâ€“Protein Interactions: The Organization and Contribution of Structurally Conserved Hot Spot Residues. Journal of Molecular Biology, 2005, 345, 1281-1294.	2.0	465
16	Amyloid Oligomers: A Joint Experimental/Computational Perspective on Alzheimerâ€™s Disease, Parkinsonâ€™s Disease, Type II Diabetes, and Amyotrophic Lateral Sclerosis. Chemical Reviews, 2021, 121, 2545-2647.	23.0	406
17	Multiple diverse ligands binding at a single protein site: A matter of pre-existing populations. Protein Science, 2009, 11, 184-197.	3.1	364
18	Studies of proteinâ€protein interfaces: A statistical analysis of the hydrophobic effect. Protein Science, 1997, 6, 53-64.	3.1	361

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19	Artificial intelligence in COVID-19 drug repurposing. The Lancet Digital Health, 2020, 2, e667-e676.	5.9	349
20	The Origin of Allosteric Functional Modulation: Multiple Pre-existing Pathways. Structure, 2009, 17, 1042-1050.	1.6	347
21	deepDR: a network-based deep learning approach toin silicodrug repositioning. Bioinformatics, 2019, 35, 5191-5198.	1.8	343
22	Folding and binding cascades: Shifts in energy landscapes. Proceedings of the National Academy of Sciences of the United States of America, 1999, 96, 9970-9972.	3.3	337
23	A Unified View of â€œHow Allostery Worksâ€• PLoS Computational Biology, 2014, 10, e1003394.	1.5	330
24	Protein Ensembles: How Does Nature Harness Thermodynamic Fluctuations for Life? The Diverse Functional Roles of Conformational Ensembles in the Cell. Chemical Reviews, 2016, 116, 6516-6551.	23.0	302
25	The Role of Protein Loops and Linkers in Conformational Dynamics and Allostery. Chemical Reviews, 2016, 116, 6391-6423.	23.0	302
26	Protein allostery, signal transmission and dynamics: a classification scheme of allosteric mechanisms. Molecular BioSystems, 2009, 5, 207.	2.9	299
27	Ras Conformational Ensembles, Allostery, and Signaling. Chemical Reviews, 2016, 116, 6607-6665.	23.0	290
28	Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578.	1.6	285
29	Polymorphism in Alzheimer Aî² Amyloid Organization Reflects Conformational Selection in a Rugged Energy Landscape. Chemical Reviews, 2010, 110, 4820-4838.	23.0	265
30	Efficient detection of three-dimensional structural motifs in biological macromolecules by computer vision techniques.. Proceedings of the National Academy of Sciences of the United States of America, 1991, 88, 10495-10499.	3.3	263
31	Conservation of polar residues as hot spots at protein interfaces. , 2000, 39, 331-342.		253
32	Allosteric Effects of the Oncogenic RasQ61L Mutant on Raf-RBD. Structure, 2015, 23, 505-516.	1.6	201
33	Dynamic Allostery: Linkers Are Not Merely Flexible. Structure, 2011, 19, 907-917.	1.6	196
34	Allostery: An Overview of Its History, Concepts, Methods, and Applications. PLoS Computational Biology, 2016, 12, e1004966.	1.5	194
35	Target identification among known drugs by deep learning from heterogeneous networks. Chemical Science, 2020, 11, 1775-1797.	3.7	193
36	Principles and Overview of Sampling Methods for Modeling Macromolecular Structure and Dynamics. PLoS Computational Biology, 2016, 12, e1004619.	1.5	188

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37	PRISM: a web server and repository for prediction of proteinâ€“protein interactions and modeling their 3D complexes. Nucleic Acids Research, 2014, 42, W285-W289.	6.5	187
38	GTP-Dependent K-Ras Dimerization. Structure, 2015, 23, 1325-1335.	1.6	187
39	Structured disorder and conformational selection. Proteins: Structure, Function and Bioinformatics, 2001, 44, 418-427.	1.5	184
40	Allostery and population shift in drug discovery. Current Opinion in Pharmacology, 2010, 10, 715-722.	1.7	176
41	Allostery without a conformational change? Revisiting the paradigm. Current Opinion in Structural Biology, 2015, 30, 17-24.	2.6	175
42	Allosteric post-translational modification codes. Trends in Biochemical Sciences, 2012, 37, 447-455.	3.7	172
43	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. Structure, 2015, 23, 1156-1167.	1.6	159
44	Topological properties of protein interaction networks from a structural perspective. Biochemical Society Transactions, 2008, 36, 1398-1403.	1.6	152
45	The Underappreciated Role of Allostery in the Cellular Network. Annual Review of Biophysics, 2013, 42, 169-189.	4.5	152
46	Drugging Ras GTPase: a comprehensive mechanistic and signaling structural view. Chemical Society Reviews, 2016, 45, 4929-4952.	18.7	150
47	The Structural Basis of Oncogenic Mutations G12, G13 and Q61 in Small GTPase K-Ras4B. Scientific Reports, 2016, 6, 21949.	1.6	149
48	A set of van der Waals and coulombic radii of protein atoms for molecular and solvent-accessible surface calculation, packing evaluation, and docking. Proteins: Structure, Function and Bioinformatics, 1998, 32, 111-127.	1.5	147
49	Electrostatic strengths of salt bridges in thermophilic and mesophilic glutamate dehydrogenase monomers. Proteins: Structure, Function and Bioinformatics, 2000, 38, 368-383.	1.5	140
50	Similar Binding Sites and Different Partners: Implications to Shared Proteins in Cellular Pathways. Structure, 2007, 15, 341-354.	1.6	136
51	Mutations in LZTR1 drive human disease by dysregulating RAS ubiquitination. Science, 2018, 362, 1177-1182.	6.0	133
52	Allo-network drugs: harnessing allostery in cellular networks. Trends in Pharmacological Sciences, 2011, 32, 686-693.	4.0	132
53	Principles of Allosteric Interactions in Cell Signaling. Journal of the American Chemical Society, 2014, 136, 17692-17701.	6.6	127
54	Computational network biology: Data, models, and applications. Physics Reports, 2020, 846, 1-66.	10.3	126

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55	A computer vision based technique for 3-D sequence-independent structural comparison of proteins. Protein Engineering, Design and Selection, 1993, 6, 279-287.	1.0	125
56	Proteinâ€“protein interaction networks: how can a hub protein bind so many different partners?. Trends in Biochemical Sciences, 2009, 34, 594-600.	3.7	125
57	Anticancer drug resistance: An update and perspective. Drug Resistance Updates, 2021, 59, 100796.	6.5	122
58	Thermodynamic Differences among Homologous Thermophilic and Mesophilic Proteins. Biochemistry, 2001, 40, 14152-14165.	1.2	119
59	Examination of shape complementarity in docking ofUnbound proteins. , 1999, 36, 307-317.		118
60	An integrated suite of fast docking algorithms. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3197-3204.	1.5	117
61	Hydrophobic folding units at proteinâ€protein interfaces: Implications to protein folding and to proteinâ€protein association. Protein Science, 1997, 6, 1426-1437.	3.1	115
62	Unraveling structural mechanisms of allosteric drug action. Trends in Pharmacological Sciences, 2014, 35, 256-264.	4.0	111
63	Protein-Protein Interfaces: Architectures and Interactions in Protein-Protein Interfaces and in Protein Cores. Their Similarities and Differences. Critical Reviews in Biochemistry and Molecular Biology, 1996, 31, 127-152.	2.3	110
64	Flexible docking allowing induced fit in proteins: Insights from an open to closed conformational isomers. Proteins: Structure, Function and Bioinformatics, 1998, 32, 159-174.	1.5	110
65	Pathogenic Autoreactive T and B Cells Cross-React with Mimotopes Expressed by a Common Human Gut Commensal to Trigger Autoimmunity. Cell Host and Microbe, 2019, 26, 100-113.e8.	5.1	109
66	PI3K inhibitors: review and new strategies. Chemical Science, 2020, 11, 5855-5865.	3.7	106
67	Multiple conformational selection and induced fit events take place in allosteric propagation. Biophysical Chemistry, 2014, 186, 22-30.	1.5	105
68	Introduction to Protein Ensembles and Allostery. Chemical Reviews, 2016, 116, 6263-6266.	23.0	105
69	Molecular surface representations by sparse critical points. Proteins: Structure, Function and Bioinformatics, 1994, 18, 94-101.	1.5	104
70	Network-based prediction of drugâ€“target interactions using an arbitrary-order proximity embedded deep forest. Bioinformatics, 2020, 36, 2805-2812.	1.8	101
71	The Different Ways through Which Specificity Works in Orthosteric and Allosteric Drugs. Current Pharmaceutical Design, 2012, 18, 1311-1316.	0.9	98
72	The Architecture of the TIR Domain Signalosome in the Toll-like Receptor-4 Signaling Pathway. Scientific Reports, 2015, 5, 13128.	1.6	98

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73	Mechanisms of Membrane Binding of Small GTPase K-Ras4B Farnesylated Hypervariable Region. Journal of Biological Chemistry, 2015, 290, 9465-9477.	1.6	98
74	The Design of Covalent Allosteric Drugs. Annual Review of Pharmacology and Toxicology, 2015, 55, 249-267.	4.2	96
75	Oncogenic Ras Isoforms Signaling Specificity at the Membrane. Cancer Research, 2018, 78, 593-602.	0.4	96
76	Synergistic Interactions between Repeats in Tau Protein and Aî² Amyloids May Be Responsible for Accelerated Aggregation via Polymorphic States. Biochemistry, 2011, 50, 5172-5181.	1.2	95
77	Membrane-associated Ras dimers are isoform-specific: K-Ras dimers differ from H-Ras dimers. Biochemical Journal, 2016, 473, 1719-1732.	1.7	92
78	Threeâ€dimensional, sequence orderâ€independent structural comparison of a serine protease against the crystallographic database reveals active site similarities: Potential implications to evolution and to protein folding. Protein Science, 1994, 3, 769-778.	3.1	90
79	A New View of Ras Isoforms in Cancers. Cancer Research, 2016, 76, 18-23.	0.4	87
80	Folding funnels and conformational transitions via hinge-bending motions. Cell Biochemistry and Biophysics, 1999, 31, 141-164.	0.9	85
81	Hydrophobic folding units derived from dissimilar monomer structures and their interactions. Protein Science, 1997, 6, 24-42.	3.1	84
82	Mechanism and evolution of protein dimerization. Protein Science, 1998, 7, 533-544.	3.1	84
83	Review: Precision medicine and driver mutations: Computational methods, functional assays and conformational principles for interpreting cancer drivers. PLoS Computational Biology, 2019, 15, e1006658.	1.5	83
84	A second molecular biology revolution? The energy landscapes of biomolecular function. Physical Chemistry Chemical Physics, 2014, 16, 6321.	1.3	82
85	Allosteric effects in the marginally stable von Hippelâ€“Lindau tumor suppressor protein and allostery-based rescue mutant design. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 901-906.	3.3	81
86	Structural Insight into Tau Proteinâ€™s Paradox of Intrinsically Disordered Behavior, Self-Acetylation Activity, and Aggregation. Journal of Physical Chemistry Letters, 2014, 5, 3026-3031.	2.1	81
87	Structural motifs at proteinâ€protein interfaces: Protein cores versus twoâ€state and threeâ€state model complexes. Protein Science, 1997, 6, 1793-1805.	3.1	78
88	Towards inferring time dimensionality in proteinâ€“protein interaction networks by integrating structures: the p53 example. Molecular BioSystems, 2009, 5, 1770.	2.9	76
89	Selective Molecular Recognition in Amyloid Growth and Transmission and Cross-Species Barriers. Journal of Molecular Biology, 2012, 421, 172-184.	2.0	76
90	The Structural Basis of ATP as an Allosteric Modulator. PLoS Computational Biology, 2014, 10, e1003831.	1.5	76

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91	An Efficient Automated Computer Vision Based Technique for Detection of Three Dimensional Structural Motifs in Proteins. Journal of Biomolecular Structure and Dynamics, 1992, 9, 769-789.	2.0	75
92	How Similar Are Protein Folding and Protein Binding Nuclei? Examination of Vibrational Motions of Energy Hot Spots and Conserved Residues. Biophysical Journal, 2005, 88, 1552-1559.	0.2	75
93	The mechanism of PI3KÎ± activation at the atomic level. Chemical Science, 2019, 10, 3671-3680.	3.7	75
94	The molecular basis of targeting protein kinases in cancer therapeutics. Seminars in Cancer Biology, 2013, 23, 235-242.	4.3	74
95	Amylinâ€“AÎ² oligomers at atomic resolution using molecular dynamics simulations: a link between Type 2 diabetes and Alzheimer's disease. Physical Chemistry Chemical Physics, 2016, 18, 2330-2338.	1.3	74
96	Transition-state Ensemble in Enzyme Catalysis: Possibility, Reality, or Necessity?. Journal of Theoretical Biology, 2000, 203, 383-397.	0.8	73
97	GTP Binding and Oncogenic Mutations May Attenuate Hypervariable Region (HVR)-Catalytic Domain Interactions in Small GTPase K-Ras4B, Exposing the Effector Binding Site. Journal of Biological Chemistry, 2015, 290, 28887-28900.	1.6	73
98	The higher level of complexity of Kâ€Ras4B activation at the membrane. FASEB Journal, 2016, 30, 1643-1655.	0.2	73
99	Surface motifs by a computer vision technique: Searches, detection, and implications for protein-ligand recognition. Proteins: Structure, Function and Bioinformatics, 1993, 16, 278-292.	1.5	72
100	The Key Role of Calmodulin in KRAS-Driven Adenocarcinomas. Molecular Cancer Research, 2015, 13, 1265-1273.	1.5	72
101	Contribution of Salt Bridges Toward Protein Thermostability. Journal of Biomolecular Structure and Dynamics, 2000, 17, 79-85.	2.0	70
102	Protein dynamics and conformational selection in bidirectional signal transduction. BMC Biology, 2012, 10, 2.	1.7	69
103	Allo-Network Drugs: Extension of the Allosteric Drug Concept to Protein- Protein Interaction and Signaling Networks. Current Topics in Medicinal Chemistry, 2013, 13, 64-77.	1.0	68
104	â€˜Latent driversâ€™ expand the cancer mutational landscape. Current Opinion in Structural Biology, 2015, 32, 25-32.	2.6	68
105	A New View of Pathway-Driven Drug Resistance in Tumor Proliferation. Trends in Pharmacological Sciences, 2017, 38, 427-437.	4.0	68
106	High-Affinity Interaction of the K-Ras4B Hypervariable Region with the Ras Active Site. Biophysical Journal, 2015, 109, 2602-2613.	0.2	67
107	Non-Redundant Unique Interface Structures as Templates for Modeling Protein Interactions. PLoS ONE, 2014, 9, e86738.	1.1	66
108	An overview of recent advances in structural bioinformatics of proteinâ€“protein interactions and a guide to their principles. Progress in Biophysics and Molecular Biology, 2014, 116, 141-150.	1.4	65

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109	Conformational Basis for Asymmetric Seeding Barrier in Filaments of Three- and Four-Repeat Tau. Journal of the American Chemical Society, 2012, 134, 10271-10278.	6.6	63
110	Cross-seeding and Conformational Selection between Three- and Four-repeat Human Tau Proteins. Journal of Biological Chemistry, 2012, 287, 14950-14959.	1.6	63
111	The Structural Pathway of Interleukin 1 (IL-1) Initiated Signaling Reveals Mechanisms of Oncogenic Mutations and SNPs in Inflammation and Cancer. PLoS Computational Biology, 2014, 10, e1003470.	1.5	63
112	MUSTA - A General, Efficient, Automated Method for Multiple Structure Alignment and Detection of Common Motifs: Application to Proteins. Journal of Computational Biology, 2001, 8, 93-121.	0.8	62
113	The structural network of inflammation and cancer: Merits and challenges. Seminars in Cancer Biology, 2013, 23, 243-251.	4.3	62
114	A Structural View of Negative Regulation of the Toll-like Receptor-Mediated Inflammatory Pathway. Biophysical Journal, 2015, 109, 1214-1226.	0.2	62
115	Inhibitors of Rasâ€“SOS Interactions. ChemMedChem, 2016, 11, 814-821.	1.6	62
116	Harnessing endophenotypes and network medicine for Alzheimer's drug repurposing. Medicinal Research Reviews, 2020, 40, 2386-2426.	5.0	61
117	Automated multiple structure alignment and detection of a common substructural motif. Proteins: Structure, Function and Bioinformatics, 2001, 43, 235-245.	1.5	60
118	Raf-1 Cysteine-Rich Domain Increases the Affinity of K-Ras/Raf at the Membrane, Promoting MAPK Signaling. Structure, 2018, 26, 513-525.e2.	1.6	60
119	Protein Folding: Binding of Conformationally Fluctuating Building Blocks Via Population Selection. Critical Reviews in Biochemistry and Molecular Biology, 2001, 36, 399-433.	2.3	58
120	The Mechanism of ATP-Dependent Allosteric Protection of Akt Kinase Phosphorylation. Structure, 2015, 23, 1725-1734.	1.6	58
121	Calmodulin and PI3K Signaling in KRAS Cancers. Trends in Cancer, 2017, 3, 214-224.	3.8	58
122	Protein ensembles link genotype to phenotype. PLoS Computational Biology, 2019, 15, e1006648.	1.5	58
123	Oncogenic KRAS signaling and YAP1/Î²-catenin: Similar cell cycle control in tumor initiation. Seminars in Cell and Developmental Biology, 2016, 58, 79-85.	2.3	54
124	â€˜Pathway drug cocktailâ€™: targeting Ras signaling based on structural pathways. Trends in Molecular Medicine, 2013, 19, 695-704.	3.5	53
125	Mechanisms of recognition of amyloid-Î² (AÎ²) monomer, oligomer, and fibril by homologous antibodies. Journal of Biological Chemistry, 2017, 292, 18325-18343.	1.6	53
126	A Systems Pharmacology Approach Uncovers Wogonoside as an Angiogenesis Inhibitor of Triple-Negative Breast Cancer by Targeting Hedgehog Signaling. Cell Chemical Biology, 2019, 26, 1143-1158.e6.	2.5	53

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127	Phosphorylated Calmodulin Promotes PI3K Activation by Binding to the SH2 Domains. Biophysical Journal, 2017, 113, 1956-1967.	0.2	51
128	Structural host-microbiota interaction networks. PLoS Computational Biology, 2017, 13, e1005579.	1.5	51
129	The quaternary assembly of KRas4B with Raf-1 at the membrane. Computational and Structural Biotechnology Journal, 2020, 18, 737-748.	1.9	50
130	A 3D sequence-independent representation of the protein data bank. Protein Engineering, Design and Selection, 1995, 8, 981-997.	1.0	49
131	Fluctuations in ion pairs and their stabilities in proteins. Proteins: Structure, Function and Bioinformatics, 2001, 43, 433-454.	1.5	48
132	Antigen binding allosterically promotes Fc receptor recognition. MAbs, 2019, 11, 58-74.	2.6	48
133	Deep learning for drug repurposing: Methods, databases, and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	48
134	Allosteric Conformational Barcodes Direct Signaling in the Cell. Structure, 2013, 21, 1509-1521.	1.6	47
135	Mapping the Conformation Space of Wildtype and Mutant H-Ras with a Memetic, Cellular, and Multiscale Evolutionary Algorithm. PLoS Computational Biology, 2015, 11, e1004470.	1.5	47
136	Personal Mutanomes Meet Modern Oncology Drug Discovery and Precision Health. Pharmacological Reviews, 2019, 71, 1-19.	7.1	47
137	Principles of docking: An overview of search algorithms and a guide to scoring functions. , 2002, 47, 409.		46
138	A broad view of scaffolding suggests that scaffolding proteins can actively control regulation and signaling of multienzyme complexes through allostery. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 820-829.	1.1	45
139	Pathogen mimicry of host protein-protein interfaces modulates immunity. Seminars in Cell and Developmental Biology, 2016, 58, 136-145.	2.3	45
140	Comparison of the Conformations of KRAS Isoforms, K-Ras4A and K-Ras4B, Points to Similarities and Significant Differences. Journal of Physical Chemistry B, 2016, 120, 667-679.	1.2	45
141	Intrinsic protein disorder in oncogenic KRAS signaling. Cellular and Molecular Life Sciences, 2017, 74, 3245-3261.	2.4	45
142	Peptideâ€“MHC (pMHC) binding to a human antiviral T cell receptor induces long-range allosteric communication between pMHC- and CD3-binding sites. Journal of Biological Chemistry, 2018, 293, 15991-16005.	1.6	45
143	The structural basis for Ras activation of PI3KÎ± lipid kinase. Physical Chemistry Chemical Physics, 2019, 21, 12021-12028.	1.3	43
144	Precision medicine review: rare driver mutations and their biophysical classification. Biophysical Reviews, 2019, 11, 5-19.	1.5	43

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145	The structural basis for cancer treatment decisions. Oncotarget, 2014, 5, 7285-7302.	0.8	43
146	Hydrophobic Interactions in the Major Groove Can Influence DNA Local Structure. Journal of Biomolecular Structure and Dynamics, 1986, 4, 41-48.	2.0	42
147	Oligomerization and nanocluster organization render specificity. Biological Reviews, 2015, 90, 587-598.	4.7	42
148	AÎ² â€œStretching-and-Packingâ€•Cross-Seeding Mechanism Can Trigger Tau Protein Aggregation. Journal of Physical Chemistry Letters, 2015, 6, 3276-3282.	2.1	42
149	Energetic redistribution in allostery to execute protein function. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 7480-7482.	3.3	41
150	Does Ras Activate Raf and PI3K Allosterically?. Frontiers in Oncology, 2019, 9, 1231.	1.3	41
151	Flexible-body motions of calmodulin and the farnesylated hypervariable region yield a high-affinity interaction enabling K-Ras4B membrane extraction. Journal of Biological Chemistry, 2017, 292, 12544-12559.	1.6	40
152	Autoinhibition in Ras effectors Raf, PI3KÎ±, and RASSF5: a comprehensive review underscoring the challenges in pharmacological intervention. Biophysical Reviews, 2018, 10, 1263-1282.	1.5	40
153	Network approaches and applications in biology. PLoS Computational Biology, 2017, 13, e1005771.	1.5	40
154	The spatial structure of cell signaling systems. Physical Biology, 2013, 10, 045004.	0.8	39
155	The free energy landscape in translational science: how can somatic mutations result in constitutive oncogenic activation?. Physical Chemistry Chemical Physics, 2014, 16, 6332.	1.3	38
156	Single Mutations in Tau Modulate the Populations of Fibril Conformers through Seed Selection. Angewandte Chemie - International Edition, 2014, 53, 1590-1593.	7.2	38
157	The disordered hypervariable region and the folded catalytic domain of oncogenic K-Ras4B partner in phospholipid binding. Current Opinion in Structural Biology, 2016, 36, 10-17.	2.6	38
158	The mechanism of activation of monomeric B-Raf V600E. Computational and Structural Biotechnology Journal, 2021, 19, 3349-3363.	1.9	38
159	Principles of K-Ras effector organization and the role of oncogenic K-Ras in cancer initiation through G1 cell cycle deregulation. Expert Review of Proteomics, 2015, 12, 669-682.	1.3	37
160	Amplification of signaling via cellular allosteric relay and protein disorder: Fig. 1.. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 6887-6888.	3.3	36
161	Unraveling the molecular mechanism of interactions of the Rho GTPases Cdc42 and Rac1 with the scaffolding protein IQGAP2. Journal of Biological Chemistry, 2018, 293, 3685-3699.	1.6	36
162	Promiscuous and specific recognition among ephrins and Eph receptors. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 1729-1740.	1.1	35

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163	Plasma membrane regulates Ras signaling networks. Cellular Logistics, 2015, 5, e1136374.	0.9	35
164	Structural disorder in four-repeat Tau fibrils reveals a new mechanism for barriers to cross-seeding of Tau isoforms. Journal of Biological Chemistry, 2018, 293, 17336-17348.	1.6	35
165	The distinct structural preferences of tau protein repeat domains. Chemical Communications, 2018, 54, 5700-5703.	2.2	35
166	Emerging Allosteric Mechanism of EGFR Activation in Physiological and Pathological Contexts. Biophysical Journal, 2019, 117, 5-13.	0.2	35
167	Is Nanoclustering essential for all oncogenic KRas pathways? Can it explain why wild-type KRas can inhibit its oncogenic variant?. Seminars in Cancer Biology, 2019, 54, 114-120.	4.3	35
168	Molecular insights into the reversible formation of tau protein fibrils. Chemical Communications, 2013, 49, 3582.	2.2	34
169	Dimerization of the SP1 Region of HIV-1 Gag Induces a Helical Conformation and Association into Helical Bundles: Implications for Particle Assembly. Journal of Virology, 2016, 90, 1773-1787.	1.5	34
170	HMI-PRED: A Web Server for Structural Prediction of Host-Microbe Interactions Based on Interface Mimicry. Journal of Molecular Biology, 2020, 432, 3395-3403.	2.0	34
171	Conformational ensembles, signal transduction and residue hot spots: application to drug discovery. Current Opinion in Drug Discovery & Development, 2010, 13, 527-37.	1.9	34
172	Gene-specific transcription activation via long-range allosteric shape-shifting. Biochemical Journal, 2011, 439, 15-25.	1.7	33
173	Atomistic-level study of the interactions between hIAPP protofibrils and membranes: Influence of pH and lipid composition. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1818-1825.	1.4	33
174	A disulphide-reinforced structural scaffold shared by small proteins with diverse functions. Nature Structural Biology, 1995, 2, 835-837.	9.7	32
175	Individualized genetic network analysis reveals new therapeutic vulnerabilities in 6,700 cancer genomes. PLoS Computational Biology, 2020, 16, e1007701.	1.5	32
176	Structural Modeling of GR Interactions with the SWI/SNF Chromatin Remodeling Complex and C/EBP. Biophysical Journal, 2015, 109, 1227-1239.	0.2	31
177	A new precision medicine initiative at the dawn of exascale computing. Signal Transduction and Targeted Therapy, 2021, 6, 3.	7.1	31
178	Flexible structural comparison allowing hinge-bending, swiveling motions. , 1999, 34, 232-254.		30
179	TRAF3 signaling: Competitive binding and evolvability of adaptive viral molecular mimicry. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 2646-2655.	1.1	30
180	The Structural Basis of the Farnesylated and Methylated KRas4B Interaction with Calmodulin. Structure, 2019, 27, 1647-1659.e4.	1.6	30

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181	The mechanism of full activation of tumor suppressor PTEN at the phosphoinositide-enriched membrane. IScience, 2021, 24, 102438.	1.9	30
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