

Ivet Bahar

List of Publications by Year in descending order

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196
papers

18,285
citations

23500

58
h-index

15218

126
g-index

217
all docs

217
docs citations

217
times ranked

17609
citing authors

#	ARTICLE	IF	CITATIONS
1	Oxidized arachidonic and adrenic PEs navigate cells to ferroptosis. <i>Nature Chemical Biology</i> , 2017, 13, 81-90.	3.9	1,589
2	Direct evaluation of thermal fluctuations in proteins using a single-parameter harmonic potential. <i>Folding & Design</i> , 1997, 2, 173-181.	4.5	1,243
3	<i>ProDy</i> : Protein Dynamics Inferred from Theory and Experiments. <i>Bioinformatics</i> , 2011, 27, 1575-1577.	1.8	907
4	Cardiolipin externalization to the outer mitochondrial membrane acts as an elimination signal for mitophagy in neuronal cells. <i>Nature Cell Biology</i> , 2013, 15, 1197-1205.	4.6	792
5	Gaussian Dynamics of Folded Proteins. <i>Physical Review Letters</i> , 1997, 79, 3090-3093.	2.9	678
6	Coarse-grained normal mode analysis in structural biology. <i>Current Opinion in Structural Biology</i> , 2005, 15, 586-592.	2.6	678
7	PEBP1 Wardens Ferroptosis by Enabling Lipoxygenase Generation of Lipid Death Signals. <i>Cell</i> , 2017, 171, 628-641.e26.	13.5	589
8	Global Dynamics of Proteins: Bridging Between Structure and Function. <i>Annual Review of Biophysics</i> , 2010, 39, 23-42.	4.5	536
9	Normal Mode Analysis of Biomolecular Structures: Functional Mechanisms of Membrane Proteins. <i>Chemical Reviews</i> , 2010, 110, 1463-1497.	23.0	461
10	Vibrational Dynamics of Folded Proteins: Significance of Slow and Fast Motions in Relation to Function and Stability. <i>Physical Review Letters</i> , 1998, 80, 2733-2736.	2.9	382
11	Structural changes involved in protein binding correlate with intrinsic motions of proteins in the unbound state. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 18908-18913.	3.3	349
12	Redox lipid reprogramming commands susceptibility of macrophages and microglia to ferroptotic death. <i>Nature Chemical Biology</i> , 2020, 16, 278-290.	3.9	299
13	Intrinsic dynamics of enzymes in the unbound state and relation to allosteric regulation. <i>Current Opinion in Structural Biology</i> , 2007, 17, 633-640.	2.6	287
14	Allostery in Its Many Disguises: From Theory to Applications. <i>Structure</i> , 2019, 27, 566-578.	1.6	285
15	Anisotropic network model: systematic evaluation and a new web interface. <i>Bioinformatics</i> , 2006, 22, 2619-2627.	1.8	279
16	Dynamics of proteins predicted by molecular dynamics simulations and analytical approaches: Application to β -amylase inhibitor. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000, 40, 512-524.	1.5	260
17	Coupling between Catalytic Site and Collective Dynamics: A Requirement for Mechanochemical Activity of Enzymes. <i>Structure</i> , 2005, 13, 893-904.	1.6	257
18	Superantigenic character of an insert unique to SARS-CoV-2 spike supported by skewed TCR repertoire in patients with hyperinflammation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 25254-25262.	3.3	252

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19	The intrinsic dynamics of enzymes plays a dominant role in determining the structural changes induced upon inhibitor binding. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 14349-14354.	3.3	248
20	Dynamics of large proteins through hierarchical levels of coarse-grained structures. Journal of Computational Chemistry, 2002, 23, 119-127.	1.5	224
21	<i>Evol</i> and <i>ProDy</i> for bridging protein sequence evolution and structural dynamics. Bioinformatics, 2014, 30, 2681-2683.	1.8	207
22	Signal Propagation in Proteins and Relation to Equilibrium Fluctuations. PLoS Computational Biology, 2007, 3, e172.	1.5	203
23	The interface of protein structure, protein biophysics, and molecular evolution. Protein Science, 2012, 21, 769-785.	3.1	188
24	Phospholipase iPLA2 ^{Î²} averts ferroptosis by eliminating a redox lipid death signal. Nature Chemical Biology, 2021, 17, 465-476.	3.9	168
25	Mapping transcriptomic vector fields of single cells. Cell, 2022, 185, 690-711.e45.	13.5	167
26	Pseudomonas aeruginosa utilizes host polyunsaturated phosphatidylethanolamines to trigger theft-ferroptosis in bronchial epithelium. Journal of Clinical Investigation, 2018, 128, 4639-4653.	3.9	159
27	The anisotropic network model web server at 2015 (ANM 2.0). Bioinformatics, 2015, 31, 1487-1489.	1.8	158
28	Predicting Drug-Target Interactions Using Probabilistic Matrix Factorization. Journal of Chemical Information and Modeling, 2013, 53, 3399-3409.	2.5	152
29	Mechanisms of CFTR Functional Variants That Impair Regulated Bicarbonate Permeation and Increase Risk for Pancreatitis but Not for Cystic Fibrosis. PLoS Genetics, 2014, 10, e1004376.	1.5	146
30	Druggability Assessment of Allosteric Proteins by Dynamics Simulations in the Presence of Probe Molecules. Journal of Chemical Theory and Computation, 2012, 8, 2435-2447.	2.3	138
31	DynOmics: dynamics of structural proteome and beyond. Nucleic Acids Research, 2017, 45, W374-W380.	6.5	135
32	Sequence Evolution Correlates with Structural Dynamics. Molecular Biology and Evolution, 2012, 29, 2253-2263.	3.5	132
33	HLA class I-associated expansion of TRBV11-2 T cells in multisystem inflammatory syndrome in children. Journal of Clinical Investigation, 2021, 131, .	3.9	130
34	Vibrational dynamics of transfer RNAs: comparison of the free and synthetase-bound forms 1 1 Edited by I. Tinoco. Journal of Molecular Biology, 1998, 281, 871-884.	2.0	126
35	Transition states and the meaning of Phi-values in protein folding kinetics. Nature Structural Biology, 2001, 8, 765-769.	9.7	125
36	Allosteric Transitions of Supramolecular Systems Explored by Network Models: Application to Chaperonin GroEL. PLoS Computational Biology, 2009, 5, e1000360.	1.5	122

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37	Principal component analysis of native ensembles of biomolecular structures (PCA_NEST): insights into functional dynamics. <i>Bioinformatics</i> , 2009, 25, 606-614.	1.8	120
38	Exploring the Conformational Transitions of Biomolecular Systems Using a Simple Two-State Anisotropic Network Model. <i>PLoS Computational Biology</i> , 2014, 10, e1003521.	1.5	112
39	Interplay between arginine methylation and ubiquitylation regulates KLF4-mediated genome stability and carcinogenesis. <i>Nature Communications</i> , 2015, 6, 8419.	5.8	107
40	Adaptability of protein structures to enable functional interactions and evolutionary implications. <i>Current Opinion in Structural Biology</i> , 2015, 35, 17-23.	2.6	104
41	ATPase Subdomain IA Is a Mediator of Interdomain Allostery in Hsp70 Molecular Chaperones. <i>PLoS Computational Biology</i> , 2014, 10, e1003624.	1.5	98
42	Common Mechanism of Pore Opening Shared by Five Different Potassium Channels. <i>Biophysical Journal</i> , 2006, 90, 3929-3940.	0.2	94
43	Toward a Molecular Understanding of the Anisotropic Response of Proteins to External Forces: Insights from Elastic Network Models. <i>Biophysical Journal</i> , 2008, 94, 3424-3435.	0.2	94
44	<i>ProDy</i> 2.0: increased scale and scope after 10 years of protein dynamics modelling with Python. <i>Bioinformatics</i> , 2021, 37, 3657-3659.	1.8	93
45	COVID-19-associated multisystem inflammatory syndrome in children (MIS-C): A novel disease that mimics toxic shock syndrome—the superantigen hypothesis. <i>Journal of Allergy and Clinical Immunology</i> , 2021, 147, 57-59.	1.5	87
46	Mechanisms of the Exchange of Diblock Copolymers between Micelles at Dynamic Equilibrium. <i>Macromolecules</i> , 1996, 29, 4764-4771.	2.2	85
47	Intrinsic dynamics is evolutionarily optimized to enable allosteric behavior. <i>Current Opinion in Structural Biology</i> , 2020, 62, 14-21.	2.6	85
48	Time-resolved Mechanism of Extracellular Gate Opening and Substrate Binding in a Glutamate Transporter. <i>Journal of Biological Chemistry</i> , 2008, 283, 28680-28690.	1.6	84
49	Pre-existing soft modes of motion uniquely defined by native contact topology facilitate ligand binding to proteins. <i>Protein Science</i> , 2011, 20, 1645-1658.	3.1	84
50	Discovery of Novel Myc ³ Max Heterodimer Disruptors with a Three-Dimensional Pharmacophore Model. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 1247-1250.	2.9	81
51	Molecular Mechanism of Dopamine Transport by Human Dopamine Transporter. <i>Structure</i> , 2015, 23, 2171-2181.	1.6	81
52	Functional Motions of Influenza Virus Hemagglutinin: A Structure-Based Analytical Approach. <i>Biophysical Journal</i> , 2002, 82, 569-581.	0.2	77
53	Mechanism of Signal Propagation upon Retinal Isomerization: Insights from Molecular Dynamics Simulations of Rhodopsin Restrained by Normal Modes. <i>Biophysical Journal</i> , 2008, 95, 789-803.	0.2	76
54	Structural dynamics is a determinant of the functional significance of missense variants. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 4164-4169.	3.3	76

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55	Cooperative Dynamics of Intact AMPA and NMDA Glutamate Receptors: Similarities and Subfamily-Specific Differences. <i>Structure</i> , 2015, 23, 1692-1704.	1.6	73
56	Complete Mapping of Substrate Translocation Highlights the Role of LeuT N-terminal Segment in Regulating Transport Cycle. <i>PLoS Computational Biology</i> , 2014, 10, e1003879.	1.5	71
57	<i>iG</i> GNM 2.0: the Gaussian network model database for biomolecular structural dynamics. <i>Nucleic Acids Research</i> , 2016, 44, D415-D422.	6.5	71
58	Monoamine transporters: structure, intrinsic dynamics and allosteric regulation. <i>Nature Structural and Molecular Biology</i> , 2019, 26, 545-556.	3.6	68
59	Resolving the paradox of ferroptotic cell death: Ferrostatin-1 binds to 15LOX/PEBP1 complex, suppresses generation of peroxidized ETE-PE, and protects against ferroptosis. <i>Redox Biology</i> , 2021, 38, 101744.	3.9	67
60	Pharmacologic Suppression of B7-H4 Glycosylation Restores Antitumor Immunity in Immune-Cold Breast Cancers. <i>Cancer Discovery</i> , 2020, 10, 1872-1893.	7.7	66
61	Coupled Global and Local Changes Direct Substrate Translocation by Neurotransmitter-Sodium Symporter Ortholog LeuT. <i>Biophysical Journal</i> , 2013, 105, 630-639.	0.2	65
62	Insights into the Modulation of Dopamine Transporter Function by Amphetamine, Orphenadrine, and Cocaine Binding. <i>Frontiers in Neurology</i> , 2015, 6, 134.	1.1	64
63	Global Transitions of Proteins Explored by a Multiscale Hybrid Methodology: Application to Adenylate Kinase. <i>Biophysical Journal</i> , 2013, 105, 1643-1652.	0.2	63
64	Empowerment of 15-Lipoxygenase Catalytic Competence in Selective Oxidation of Membrane ETE-PE to Ferroptotic Death Signals, HpETE-PE. <i>Journal of the American Chemical Society</i> , 2018, 140, 17835-17839.	6.6	63
65	Rhapsody: predicting the pathogenicity of human missense variants. <i>Bioinformatics</i> , 2020, 36, 3084-3092.	1.8	63
66	Regulation of XIAP Turnover Reveals a Role for USP11 in Promotion of Tumorigenesis. <i>EBioMedicine</i> , 2017, 15, 48-61.	2.7	61
67	Development of Small-Molecule PUMA Inhibitors for Mitigating Radiation-Induced Cell Death. <i>Current Topics in Medicinal Chemistry</i> , 2011, 11, 281-290.	1.0	57
68	PEBP1 acts as a rheostat between prosurvival autophagy and ferroptotic death in asthmatic epithelial cells. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 14376-14385.	3.3	57
69	Multisystem Inflammatory Syndrome in Children and Long COVID: The SARS-CoV-2 Viral Superantigen Hypothesis. <i>Frontiers in Immunology</i> , 0, 13, .	2.2	56
70	Large collective motions regulate the functional properties of glutamate transporter trimers. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 15141-15146.	3.3	55
71	Structure-Encoded Global Motions and Their Role in Mediating Protein-Substrate Interactions. <i>Biophysical Journal</i> , 2015, 109, 1101-1109.	0.2	55
72	Allosteric Modulation of Intact $\hat{3}$ -Secretase Structural Dynamics. <i>Biophysical Journal</i> , 2017, 113, 2634-2649.	0.2	55

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73	Dynamics and allosteric potential of the AMPA receptor N-terminal domain. <i>EMBO Journal</i> , 2011, 30, 972-982.	3.5	53
74	On the functional significance of soft modes predicted by coarse-grained models for membrane proteins. <i>Journal of General Physiology</i> , 2010, 135, 563-573.	0.9	49
75	Molecular simulations elucidate the substrate translocation pathway in a glutamate transporter. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 2589-2594.	3.3	48
76	Microseconds Simulations Reveal a New Sodium-binding Site and the Mechanism of Sodium-coupled Substrate Uptake by LeuT. <i>Journal of Biological Chemistry</i> , 2015, 290, 544-555.	1.6	48
77	Constraints Imposed by the Membrane Selectively Guide the Alternating Access Dynamics of the Glutamate Transporter GltPh. <i>Biophysical Journal</i> , 2012, 102, 1331-1340.	0.2	47
78	Innate immune memory and homeostasis may be conferred through crosstalk between the TLR3 and TLR7 pathways. <i>Science Signaling</i> , 2016, 9, ra70.	1.6	46
79	A Perspective on Implementing a Quantitative Systems Pharmacology Platform for Drug Discovery and the Advancement of Personalized Medicine. <i>Journal of Biomolecular Screening</i> , 2016, 21, 521-534.	2.6	46
80	Shared Signature Dynamics Tempered by Local Fluctuations Enables Fold Adaptability and Specificity. <i>Molecular Biology and Evolution</i> , 2019, 36, 2053-2068.	3.5	45
81	The mechanism of substrate release by the aspartate transporter Glt _{Ph} : insights from simulations. <i>Molecular BioSystems</i> , 2011, 7, 832-842.	2.9	44
82	ClustENM: ENM-Based Sampling of Essential Conformational Space at Full Atomic Resolution. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4549-4562.	2.3	43
83	Spatial bias in cAMP generation determines biological responses to PTH type 1 receptor activation. <i>Science Signaling</i> , 2021, 14, eabc5944.	1.6	43
84	Quantitative assessment of cell fate decision between autophagy and apoptosis. <i>Scientific Reports</i> , 2017, 7, 17605.	1.6	42
85	On the Conservation of the Slow Conformational Dynamics within the Amino Acid Kinase Family: NAGK the Paradigm. <i>PLoS Computational Biology</i> , 2010, 6, e1000738.	1.5	41
86	A genome-wide RNAi screen identifies potential drug targets in a <i>C. elegans</i> model of α 1-antitrypsin deficiency. <i>Human Molecular Genetics</i> , 2014, 23, 5123-5132.	1.4	41
87	Significance of p53 dynamics in regulating apoptosis in response to ionizing radiation and polypharmacological strategies. <i>Scientific Reports</i> , 2014, 4, 6245.	1.6	41
88	Designing inhibitors of cytochrome c/cardiolipin peroxidase complexes: mitochondria-targeted imidazole-substituted fatty acids. <i>Free Radical Biology and Medicine</i> , 2014, 71, 221-230.	1.3	40
89	Intracellular Gating in an Inward-facing State of Aspartate Transporter GltPh Is Regulated by the Movements of the Helical Hairpin HP2. <i>Journal of Biological Chemistry</i> , 2013, 288, 8231-8237.	1.6	39
90	Residue packing in proteins: Uniform distribution on a coarse-grained scale. <i>Journal of Chemical Physics</i> , 2002, 116, 2269-2276.	1.2	38

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91	Allosteric interactions in the parathyroid hormone GPCRâ€‘arrestin complex formation. <i>Nature Chemical Biology</i> , 2020, 16, 1096-1104.	3.9	38
92	Anti-Ferroptosis Drug Enhances Total-Body Irradiation Mitigation by Drugs that Block Apoptosis and Necroptosis. <i>Radiation Research</i> , 2020, 193, 435.	0.7	36
93	Essential site scanning analysis: A new approach for detecting sites that modulate the dispersion of protein global motions. <i>Computational and Structural Biotechnology Journal</i> , 2020, 18, 1577-1586.	1.9	35
94	Comparative Dynamics of NMDA- and AMPA-Glutamate Receptor N-Terminal Domains. <i>Structure</i> , 2012, 20, 1838-1849.	1.6	34
95	Energy landscape of LeuT from molecular simulations. <i>Journal of Chemical Physics</i> , 2015, 143, 243134.	1.2	34
96	PINK1 Interacts with VCP/p97 and Activates PKA to Promote NSFL1C/p47 Phosphorylation and Dendritic Arborization in Neurons. <i>ENeuro</i> , 2018, 5, ENEURO.0466-18.2018.	0.9	34
97	Characterization of Differential Dynamics, Specificity, and Allostery of Lipoxygenase Family Members. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2496-2508.	2.5	34
98	â€‘Only a Life Lived for Others Is Worth Livingâ€‘: Redox Signaling by Oxygenated Phospholipids in Cell Fate Decisions. <i>Antioxidants and Redox Signaling</i> , 2018, 29, 1333-1358.	2.5	33
99	A novel strategy to block mitotic progression for targeted therapy. <i>EBioMedicine</i> , 2019, 49, 40-54.	2.7	33
100	Towards gaining sight of multiscale events: utilizing network models and normal modes in hybrid methods. <i>Current Opinion in Structural Biology</i> , 2020, 64, 34-41.	2.6	32
101	Impact of new variants on SARS-CoV-2 infectivity and neutralization: A molecular assessment of the alterations in the spike-host protein interactions. <i>IScience</i> , 2022, 25, 103939.	1.9	32
102	The center for causal discovery of biomedical knowledge from big data. <i>Journal of the American Medical Informatics Association: JAMIA</i> , 2015, 22, 1132-1136.	2.2	30
103	Pore dilatation increases the bicarbonate permeability of CFTR, ANO1 and glycine receptor anion channels. <i>Journal of Physiology</i> , 2016, 594, 2929-2955.	1.3	30
104	HiDeF: identifying persistent structures in multiscale â€‘omics data. <i>Genome Biology</i> , 2021, 22, 21.	3.8	29
105	BalestraWeb: efficient online evaluation of drugâ€‘target interactions. <i>Bioinformatics</i> , 2015, 31, 131-133.	1.8	28
106	A monoclonal antibody against staphylococcal enterotoxin B superantigen inhibits SARS-CoV-2 entry in vitro. <i>Structure</i> , 2021, 29, 951-962.e3.	1.6	28
107	Structure, Dynamics, and Allosteric Potential of Ionotropic Glutamate Receptor N-Terminal Domains. <i>Biophysical Journal</i> , 2015, 109, 1136-1148.	0.2	27
108	Improved Total-Body Irradiation Survival by Delivery of Two Radiation Mitigators that Target Distinct Cell Death Pathways. <i>Radiation Research</i> , 2017, 189, 68.	0.7	27

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109	A novel small-molecule antagonizes PRMT5-mediated KLF4 methylation for targeted therapy. <i>EBioMedicine</i> , 2019, 44, 98-111.	2.7	27
110	Regulation of CFTR Bicarbonate Channel Activity by WNK1: Implications for Pancreatitis and CFTR-Related Disorders. <i>Cellular and Molecular Gastroenterology and Hepatology</i> , 2020, 9, 79-103.	2.3	27
111	A network of phosphatidylinositol (4,5)-bisphosphate (PIP2) binding sites on the dopamine transporter regulates amphetamine behavior in <i>Drosophila Melanogaster</i> . <i>Molecular Psychiatry</i> , 2021, 26, 4417-4430.	4.1	26
112	Substrate transport and anion permeation proceed through distinct pathways in glutamate transporters. <i>ELife</i> , 2017, 6, .	2.8	26
113	Quantitative Assessment of the Energetics of Dopamine Translocation by Human Dopamine Transporter. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5336-5346.	1.2	25
114	Recruitment of pro-IL-1 β to mitochondrial cardiolipin, via shared LC3 binding domain, inhibits mitophagy and drives maximal NLRP3 activation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	25
115	Cooperative dynamics of proteins unraveled by network models. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 426-439.	6.2	24
116	Chromosomal dynamics predicted by an elastic network model explains genome-wide accessibility and long-range couplings. <i>Nucleic Acids Research</i> , 2017, 45, 3663-3673.	6.5	24
117	Shared dynamics of LeuT superfamily members and allosteric differentiation by structural irregularities and multimerization. <i>Philosophical Transactions of the Royal Society B: Biological Sciences</i> , 2018, 373, 20170177.	1.8	24
118	EIF3H Orchestrates Hippo Pathway-Mediated Oncogenesis via Catalytic Control of YAP Stability. <i>Cancer Research</i> , 2020, 80, 2550-2563.	0.4	24
119	Allosteric modulation of human dopamine transporter activity under conditions promoting its dimerization. <i>Journal of Biological Chemistry</i> , 2017, 292, 12471-12482.	1.6	23
120	QuartataWeb: Integrated Chemical-Protein-Pathway Mapping for Polypharmacology and Chemogenomics. <i>Bioinformatics</i> , 2020, 36, 3935-3937.	1.8	23
121	Comparative study of the effectiveness and limitations of current methods for detecting sequence coevolution. <i>Bioinformatics</i> , 2015, 31, 1929-1937.	1.8	22
122	Connecting Neuronal Cell Protective Pathways and Drug Combinations in a Huntington's Disease Model through the Application of Quantitative Systems Pharmacology. <i>Scientific Reports</i> , 2017, 7, 17803.	1.6	22
123	A systems-level study reveals host-targeted repurposable drugs against SARS-CoV-2 infection. <i>Molecular Systems Biology</i> , 2021, 17, e10239.	3.2	22
124	Markov Methods for Hierarchical Coarse-Graining of Large Protein Dynamics. <i>Journal of Computational Biology</i> , 2007, 14, 765-776.	0.8	21
125	FlexE: Using Elastic Network Models to Compare Models of Protein Structure. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3985-3991.	2.3	20
126	Effect of Dimerization on the Dynamics of Neurotransmitter:Sodium Symporters. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3657-3666.	1.2	20

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127	Key residues controlling bidirectional ion movements in Na ⁺ /Ca ²⁺ exchanger. <i>Cell Calcium</i> , 2018, 76, 10-22.	1.1	20
128	Protonation of Glutamate 208 Induces the Release of Agmatine in an Outward-facing Conformation of an Arginine/Agmatine Antiporter. <i>Journal of Biological Chemistry</i> , 2011, 286, 19693-19701.	1.6	19
129	Inhibition of Peroxidase Activity of Cytochrome <i>c</i> : De Novo Compound Discovery and Validation. <i>Molecular Pharmacology</i> , 2015, 88, 421-427.	1.0	19
130	An analog of glibenclamide selectively enhances autophagic degradation of misfolded Î±1-antitrypsin Z. <i>PLoS ONE</i> , 2019, 14, e0209748.	1.1	19
131	Pharmmaker: Pharmacophore modeling and hit identification based on druggability simulations. <i>Protein Science</i> , 2020, 29, 76-86.	3.1	19
132	NO ²⁻ Represses the Oxygenation of Arachidonoyl PE by 15LOX/PEBP1: Mechanism and Role in Ferroptosis. <i>International Journal of Molecular Sciences</i> , 2021, 22, 5253.	1.8	19
133	Computer simulations of two-dimensional trifunctional bimodal networks. <i>Macromolecular Theory and Simulations</i> , 1994, 3, 151-161.	0.6	17
134	A Conformational Switch in a Partially Unwound Helix Selectively Determines the Pathway for Substrate Release from the Carnitine/ ³ -Butyrobetaine Antiporter CaiT. <i>Journal of Biological Chemistry</i> , 2012, 287, 31823-31832.	1.6	17
135	Nanomechanics of multidomain neuronal cell adhesion protein contactin revealed by single molecule AFM and SMD. <i>Scientific Reports</i> , 2017, 7, 8852.	1.6	17
136	Mechanisms of Action of Autophagy Modulators Dissected by Quantitative Systems Pharmacology Analysis. <i>International Journal of Molecular Sciences</i> , 2020, 21, 2855.	1.8	17
137	Targeting of dopamine transporter to filopodia requires an outward-facing conformation of the transporter. <i>Scientific Reports</i> , 2017, 7, 5399.	1.6	16
138	Druggability Simulations and X-Ray Crystallography Reveal a Ligand-Binding Site in the GluA3 AMPA Receptor N-Terminal Domain. <i>Structure</i> , 2019, 27, 241-252.e3.	1.6	16
139	Anisotropy of static and dynamic orientational correlations in N-alkanes. <i>Journal of Chemical Physics</i> , 1988, 88, 1228-1234.	1.2	15
140	Inactivation of RIP3 kinase sensitizes to 15LOX/PEBP1-mediated ferroptotic death. <i>Redox Biology</i> , 2022, 50, 102232.	3.9	15
141	Dynamic Modulation of Binding Affinity as a Mechanism for Regulating Interferon Signaling. <i>Journal of Molecular Biology</i> , 2017, 429, 2571-2589.	2.0	14
142	Harnessing Human Microphysiology Systems as Key Experimental Models for Quantitative Systems Pharmacology. <i>Handbook of Experimental Pharmacology</i> , 2019, 260, 327-367.	0.9	14
143	New insight into the significance of KLF4 PARylation in genome stability, carcinogenesis, and therapy. <i>EMBO Molecular Medicine</i> , 2020, 12, e12391.	3.3	14
144	Sampling of Protein Conformational Space Using Hybrid Simulations: A Critical Assessment of Recent Methods. <i>Frontiers in Molecular Biosciences</i> , 2022, 9, 832847.	1.6	14

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145	Psychomotor impairments and therapeutic implications revealed by a mutation associated with infantile Parkinsonism-Dystonia. <i>ELife</i> , 2021, 10, .	2.8	13
146	State-dependent sequential allostery exhibited by chaperonin TRiC/CCT revealed by network analysis of Cryo-EM maps. <i>Progress in Biophysics and Molecular Biology</i> , 2021, 160, 104-120.	1.4	12
147	Orientalional and conformational correlations in deformed polymer chains with fixed end-to-end separation: A Brownian dynamics simulation study. <i>Journal of Chemical Physics</i> , 1992, 97, 4428-4437.	1.2	11
148	Activation and desensitization of ionotropic glutamate receptors by selectively triggering pre-existing motions. <i>Neuroscience Letters</i> , 2019, 700, 22-29.	1.0	11
149	Adaptability and specificity: how do proteins balance opposing needs to achieve function?. <i>Current Opinion in Structural Biology</i> , 2021, 67, 25-32.	2.6	11
150	ClustENMD: efficient sampling of biomolecular conformational space at atomic resolution. <i>Bioinformatics</i> , 2021, 37, 3956-3958.	1.8	11
151	Elastic Network Models For Biomolecular Dynamics: Theory and Application to Membrane Proteins and Viruses. <i>World Scientific Lecture Notes in Complex Systems</i> , 2009, , 129-158.	0.1	11
152	Precise druggability of the PTH type 1 receptor. <i>Nature Chemical Biology</i> , 2022, 18, 272-280.	3.9	11
153	Quantitative Systems Pharmacological Analysis of Drugs of Abuse Reveals the Pleiotropy of Their Targets and the Effector Role of mTORC1. <i>Frontiers in Pharmacology</i> , 2019, 10, 191.	1.6	10
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