Ivet Bahar

List of Publications by Year in Descending Order

180 papers	12,825 citations	51 h-index	111 g-index
217 ext. papers	15,796 ext. citations	7.2 avg, IF	6.76 L-index

#	Paper	IF	Citations
180	Mapping transcriptomic vector fields of single cells.. *Cell*, **2022**,	56.2	9
179	Sampling of Protein Conformational Space Using Hybrid Simulations: A Critical Assessment of Recent Methods.. *Frontiers in Molecular Biosciences*, **2022**, 9, 832847	5.6	2
178	Inactivation of RIP3 kinase sensitizes to 15LOX/PEBP1-mediated ferroptotic death.. *Redox Biology*, **2022**, 50, 102232	11.3	1
177	Impact of new variants on SARS-CoV-2 infectivity and neutralization: A molecular assessment of the alterations in the spike-host protein interactions.. *IScience*, **2022**, 25, 103939	6.1	2
176	Protein dynamics developments for the large scale and cryoEM: case study of ProDy 2.0.. *Acta Crystallographica Section D: Structural Biology*, **2022**, 78, 399-409	5.5	1
175	Approximating deformation fields for the analysis of continuous heterogeneity of biological macromolecules by 3D Zernike polynomials. *IUCrJ*, **2021**, 8, 992-1005	4.7	1
174	Spatial bias in cAMP generation determines biological responses to PTH type 1 receptor activation. *Science Signaling*, **2021**, 14, eabc5944	8.8	4
173	Recruitment of pro-IL-1β to mitochondrial cardiolipin, via shared LC3 binding domain, inhibits mitophagy and drives maximal NLRP3 activation. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	7
172	HLA class I-associated expansion of TRBV11-2 T cells in multisystem inflammatory syndrome in children. *Journal of Clinical Investigation*, **2021**, 131,	15.9	39
171	Predicting Protein-Protein Interactions Using Symmetric Logistic Matrix Factorization. *Journal of Chemical Information and Modeling*, **2021**, 61, 1670-1682	6.1	2
170	ProDy 2.0: Increased Scale and Scope after 10 Years of Protein Dynamics Modelling with Python. *Bioinformatics*, **2021**,	7.2	20
169	NO Represses the Oxygenation of Arachidonoyl PE by 15LOX/PEBP1: Mechanism and Role in Ferroptosis. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	4
168	Normal mode analysis of membrane protein dynamics using the vibrational subsystem analysis. *Journal of Chemical Physics*, **2021**, 154, 195102	3.9	2
167	Psychomotor impairments and therapeutic implications revealed by a mutation associated with infantile Parkinsonism-Dystonia. *ELife*, **2021**, 10,	8.9	5
166	Functional Characterization of the Dopaminergic Psychostimulant Sydnocarb as an Allosteric Modulator of the Human Dopamine Transporter. *Biomedicines*, **2021**, 9,	4.8	3
165	A network of phosphatidylinositol (4,5)-bisphosphate (PIP) binding sites on the dopamine transporter regulates amphetamine behavior in Drosophila Melanogaster. *Molecular Psychiatry*, **2021**, 26, 4417-4430	15.1	10
164	State-dependent sequential allostery exhibited by chaperonin TRiC/CCT revealed by network analysis of Cryo-EM maps. *Progress in Biophysics and Molecular Biology*, **2021**, 160, 104-120	4.7	5

163	Resolving the paradox of ferroptotic cell death: Ferrostatin-1 binds to 15LOX/PEBP1 complex, suppresses generation of peroxidized ETE-PE, and protects against ferroptosis. *Redox Biology*, **2021**, 38, 101744	11.3	23
162	Adaptability and specificity: how do proteins balance opposing needs to achieve function?. *Current Opinion in Structural Biology*, **2021**, 67, 25-32	8.1	5
161	Direct coupling of oligomerization and oligomerization-driven endocytosis of the dopamine transporter to its conformational mechanics and activity. *Journal of Biological Chemistry*, **2021**, 296, 100430	5.4	2
160	Phospholipase iPLA□averts ferroptosis by eliminating a redox lipid death signal. *Nature Chemical Biology*, **2021**, 17, 465-476	11.7	31
159	Coupled mixed model for joint genetic analysis of complex disorders with two independently collected data sets. *BMC Bioinformatics*, **2021**, 22, 50	3.6	0
158	ClustENMD: Efficient sampling of biomolecular conformational space at atomic resolution. *Bioinformatics*, **2021**,	7.2	3
157	A systems-level study reveals host-targeted repurposable drugs against SARS-CoV-2 infection. *Molecular Systems Biology*, **2021**, 17, e10239	12.2	5
156	A monoclonal antibody against staphylococcal enterotoxin B superantigen inhibits SARS-CoV-2 entry in□vitro. *Structure*, **2021**, 29, 951-962.e3	5.2	13
155	HiDeF: identifying persistent structures in multiscale 'omics data. *Genome Biology*, **2021**, 22, 21	18.3	11
154	Allosteric Modulator KM822 Attenuates Behavioral Actions of Amphetamine in C. elegans through Interactions with the Dopamine Transporter DAT-1.. *Molecular Pharmacology*, **2021**,	4.3	1
153	Bile Acids Gate Dopamine Transporter Mediated Currents.. *Frontiers in Chemistry*, **2021**, 9, 753990	5	0
152	Essential site scanning analysis: A new approach for detecting sites that modulate the dispersion of protein global motions. *Computational and Structural Biotechnology Journal*, **2020**, 18, 1577-1586	6.8	13
151	PEBP1 acts as a rheostat between prosurvival autophagy and ferroptotic death in asthmatic epithelial cells. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 14376-14385	11.5	27
150	Allosteric interactions in the parathyroid hormone GPCR-arrestin complex formation. *Nature Chemical Biology*, **2020**, 16, 1096-1104	11.7	16
149	Rhapsody: predicting the pathogenicity of human missense variants. *Bioinformatics*, **2020**, 36, 3084-3092	7.2	28
148	Modulation of Toroidal Proteins Dynamics in Favor of Functional Mechanisms upon Ligand Binding. *Biophysical Journal*, **2020**, 118, 1782-1794	2.9	4
147	Redox lipid reprogramming commands susceptibility of macrophages and microglia to ferroptotic death. *Nature Chemical Biology*, **2020**, 16, 278-290	11.7	105
146	Allostery as Structure-Encoded Collective Dynamics **2020**, 125-141		1

145	Mechanisms of Action of Autophagy Modulators Dissected by Quantitative Systems Pharmacology Analysis. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	8
144	Anti-Ferroptosis Drug Enhances Total-Body Irradiation Mitigation by Drugs that Block Apoptosis and Necroptosis. *Radiation Research*, **2020**, 193, 435-450	3.1	20
143	New insight into the significance of KLF4 PARylation in genome stability, carcinogenesis, and therapy. *EMBO Molecular Medicine*, **2020**, 12, e12391	12	5
142	An insertion unique to SARS-CoV-2 exhibits superantigenic character strengthened by recent mutations **2020**,		21
141	Identification of a unique TCR repertoire, consistent with a superantigen selection process in Children with Multi-system Inflammatory Syndrome **2020**,		5
140	A monoclonal antibody against staphylococcal enterotoxin B superantigen inhibits SARS-CoV-2 entry **2020**,		6
139	Pharmmaker: Pharmacophore modeling and hit identification based on druggability simulations. *Protein Science*, **2020**, 29, 76-86	6.3	14
138	Differences in the intrinsic spatial dynamics of the chromatin contribute to cell differentiation. *Nucleic Acids Research*, **2020**, 48, 1131-1145	20.1	4
137	Intrinsic dynamics is evolutionarily optimized to enable allosteric behavior. *Current Opinion in Structural Biology*, **2020**, 62, 14-21	8.1	39
136	Superantigenic character of an insert unique to SARS-CoV-2 spike supported by skewed TCR repertoire in patients with hyperinflammation. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 25254-25262	11.5	116
135	Towards gaining sight of multiscale events: utilizing network models and normal modes in hybrid methods. *Current Opinion in Structural Biology*, **2020**, 64, 34-41	8.1	13
134	Pharmacologic Suppression of B7-H4 Glycosylation Restores Antitumor Immunity in Immune-Cold Breast Cancers. *Cancer Discovery*, **2020**, 10, 1872-1893	24.4	21
133	Regulation of CFTR Bicarbonate Channel Activity by WNK1: Implications for Pancreatitis and CFTR-Related Disorders. *Cellular and Molecular Gastroenterology and Hepatology*, **2020**, 9, 79-103	7.9	15
132	QuartataWeb: Integrated Chemical-Protein-Pathway Mapping for Polypharmacology and Chemogenomics. *Bioinformatics*, **2020**, 36, 3935-3937	7.2	10
131	EIF3H Orchestrates Hippo Pathway-Mediated Oncogenesis via Catalytic Control of YAP Stability. *Cancer Research*, **2020**, 80, 2550-2563	10.1	9
130	Complementary computational and experimental evaluation of missense variants in the ROMK potassium channel. *PLoS Computational Biology*, **2020**, 16, e1007749	5	1
129	Druggability Simulations and X-Ray Crystallography Reveal a Ligand-Binding Site in the GluA3 AMPA Receptor N-Terminal Domain. *Structure*, **2019**, 27, 241-252.e3	5.2	11
128	Trimerization of dopamine transporter triggered by AIM-100 binding: Molecular mechanism and effect of mutations. *Neuropharmacology*, **2019**, 161, 107676	5.5	5

127	Harnessing Human Microphysiology Systems as Key Experimental Models for Quantitative Systems Pharmacology. *Handbook of Experimental Pharmacology*, **2019**, 260, 327-367	3.2	9
126	A novel small-molecule antagonizes PRMT5-mediated KLF4 methylation for targeted therapy. *EBioMedicine*, **2019**, 44, 98-111	8.8	13
125	Shared Signature Dynamics Tempered by Local Fluctuations Enables Fold Adaptability and Specificity. *Molecular Biology and Evolution*, **2019**, 36, 2053-2068	8.3	26
124	Quantitative Systems Pharmacological Analysis of Drugs of Abuse Reveals the Pleiotropy of Their Targets and the Effector Role of mTORC1. *Frontiers in Pharmacology*, **2019**, 10, 191	5.6	6
123	An analog of glibenclamide selectively enhances autophagic degradation of misfolded 1-antitrypsin Z. *PLoS ONE*, **2019**, 14, e0209748	3.7	11
122	Allostery in Its Many Disguises: From Theory to Applications. *Structure*, **2019**, 27, 566-578	5.2	158
121	Radioresistance of Serpinb3a-/- Mice and Derived Hematopoietic and Marrow Stromal Cell Lines. *Radiation Research*, **2019**, 192, 267-281	3.1	2
120	Monoamine transporters: structure, intrinsic dynamics and allosteric regulation. *Nature Structural and Molecular Biology*, **2019**, 26, 545-556	17.6	40
119	A novel strategy to block mitotic progression for targeted therapy. *EBioMedicine*, **2019**, 49, 40-54	8.8	17
118	Characterization of Differential Dynamics, Specificity, and Allostery of Lipoxygenase Family Members. *Journal of Chemical Information and Modeling*, **2019**, 59, 2496-2508	6.1	18
117	Activation and desensitization of ionotropic glutamate receptors by selectively triggering pre-existing motions. *Neuroscience Letters*, **2019**, 700, 22-29	3.3	8
116	Structural dynamics is a determinant of the functional significance of missense variants. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 4164-4169	11.5	45
115	"Only a Life Lived for Others Is Worth Living": Redox Signaling by Oxygenated Phospholipids in Cell Fate Decisions. *Antioxidants and Redox Signaling*, **2018**, 29, 1333-1358	8.4	20
114	Improved Total-Body Irradiation Survival by Delivery of Two Radiation Mitigators that Target Distinct Cell Death Pathways. *Radiation Research*, **2018**, 189, 68-83	3.1	20
113	Heterogeneities in Axonal Structure and Transporter Distribution Lower Dopamine Reuptake Efficiency. *ENeuro*, **2018**, 5,	3.9	8
112	Quantitative Assessment of the Energetics of Dopamine Translocation by Human Dopamine Transporter. *Journal of Physical Chemistry B*, **2018**, 122, 5336-5346	3.4	17
111	PINK1 Interacts with VCP/p97 and Activates PKA to Promote NSFL1C/p47 Phosphorylation and Dendritic Arborization in Neurons. *ENeuro*, **2018**, 5,	3.9	24
110	Empowerment of 15-Lipoxygenase Catalytic Competence in Selective Oxidation of Membrane ETE-PE to Ferroptotic Death Signals, HpETE-PE. *Journal of the American Chemical Society*, **2018**, 140, 17835-17839	16.4	38

109	Key residues controlling bidirectional ion movements in Na/Ca exchanger. *Cell Calcium*, **2018**, 76, 10-22	4	15
108	Pseudomonas aeruginosa utilizes host polyunsaturated phosphatidylethanolamines to trigger theft-ferroptosis in bronchial epithelium. *Journal of Clinical Investigation*, **2018**, 128, 4639-4653	15.9	71
107	Shared dynamics of LeuT superfamily members and allosteric differentiation by structural irregularities and multimerization. *Philosophical Transactions of the Royal Society B: Biological Sciences*, **2018**, 373,	5.8	18
106	Effect of Dimerization on the Dynamics of Neurotransmitter:Sodium Symporters. *Journal of Physical Chemistry B*, **2017**, 121, 3657-3666	3.4	13
105	Chromosomal dynamics predicted by an elastic network model explains genome-wide accessibility and long-range couplings. *Nucleic Acids Research*, **2017**, 45, 3663-3673	20.1	13
104	Allosteric modulation of human dopamine transporter activity under conditions promoting its dimerization. *Journal of Biological Chemistry*, **2017**, 292, 12471-12482	5.4	16
103	Regulation of XIAP Turnover Reveals a Role for USP11 in Promotion of Tumorigenesis. *EBioMedicine*, **2017**, 15, 48-61	8.8	40
102	PEBP1 Wardens Ferroptosis by Enabling Lipoxygenase Generation of Lipid Death Signals. *Cell*, **2017**, 171, 628-641.e26	56.2	321
101	Nanomechanics of multidomain neuronal cell adhesion protein contactin revealed by single molecule AFM and SMD. *Scientific Reports*, **2017**, 7, 8852	4.9	12
100	Targeting of dopamine transporter to filopodia requires an outward-facing conformation of the transporter. *Scientific Reports*, **2017**, 7, 5399	4.9	13
99	Quantitative assessment of cell fate decision between autophagy and apoptosis. *Scientific Reports*, **2017**, 7, 17605	4.9	25
98	Dynamic Modulation of Binding Affinity as a Mechanism for Regulating Interferon Signaling. *Journal of Molecular Biology*, **2017**, 429, 2571-2589	6.5	10
97	Oxidized arachidonic and adrenic PEs navigate cells to ferroptosis. *Nature Chemical Biology*, **2017**, 13, 81-90	11.7	754
96	Allosteric Modulation of Intact -Secretase Structural Dynamics. *Biophysical Journal*, **2017**, 113, 2634-2649	2.9	27
95	Connecting Neuronal Cell Protective Pathways and Drug Combinations in a Huntington's Disease Model through the Application of Quantitative Systems Pharmacology. *Scientific Reports*, **2017**, 7, 17803	4.9	13
94	DynOmics: dynamics of structural proteome and beyond. *Nucleic Acids Research*, **2017**, 45, W374-W380	20.1	92
93	Substrate transport and anion permeation proceed through distinct pathways in glutamate transporters. *ELife*, **2017**, 6,	8.9	16
92	Innate immune memory and homeostasis may be conferred through crosstalk between the TLR3 and TLR7 pathways. *Science Signaling*, **2016**, 9, ra70	8.8	25

91	A Perspective on Implementing a Quantitative Systems Pharmacology Platform for Drug Discovery and the Advancement of Personalized Medicine. *Journal of Biomolecular Screening*, **2016**, 21, 521-34		29
90	iGNM 2.0: the Gaussian network model database for biomolecular structural dynamics. *Nucleic Acids Research*, **2016**, 44, D415-22	20.1	59
89	Pore dilatation increases the bicarbonate permeability of CFTR, ANO1 and glycine receptor anion channels. *Journal of Physiology*, **2016**, 594, 2929-55	3.9	24
88	ClustENM: ENM-Based Sampling of Essential Conformational Space at Full Atomic Resolution. *Journal of Chemical Theory and Computation*, **2016**, 12, 4549-62	6.4	27
87	Adaptability of protein structures to enable functional interactions and evolutionary implications. *Current Opinion in Structural Biology*, **2015**, 35, 17-23	8.1	79
86	Inhibition of Peroxidase Activity of Cytochrome c: De Novo Compound Discovery and Validation. *Molecular Pharmacology*, **2015**, 88, 421-7	4.3	19
85	The center for causal discovery of biomedical knowledge from big data. *Journal of the American Medical Informatics Association: JAMIA*, **2015**, 22, 1132-6	8.6	21
84	Structure-Encoded Global Motions and Their Role in Mediating Protein-Substrate Interactions. *Biophysical Journal*, **2015**, 109, 1101-9	2.9	39
83	BalestraWeb: efficient online evaluation of drug-target interactions. *Bioinformatics*, **2015**, 31, 131-3	7.2	18
82	Molecular Mechanism of Dopamine Transport by Human Dopamine Transporter. *Structure*, **2015**, 23, 2171-81	5.2	57
81	Interplay between arginine methylation and ubiquitylation regulates KLF4-mediated genome stability and carcinogenesis. *Nature Communications*, **2015**, 6, 8419	17.4	74
80	Cooperative Dynamics of Intact AMPA and NMDA Glutamate Receptors: Similarities and Subfamily-Specific Differences. *Structure*, **2015**, 23, 1692-1704	5.2	53
79	The anisotropic network model web server at 2015 (ANM 2.0). *Bioinformatics*, **2015**, 31, 1487-9	7.2	118
78	Energy landscape of LeuT from molecular simulations. *Journal of Chemical Physics*, **2015**, 143, 243134	3.9	28
77	Insights into the Modulation of Dopamine Transporter Function by Amphetamine, Orphenadrine, and Cocaine Binding. *Frontiers in Neurology*, **2015**, 6, 134	4.1	49
76	Microseconds simulations reveal a new sodium-binding site and the mechanism of sodium-coupled substrate uptake by LeuT. *Journal of Biological Chemistry*, **2015**, 290, 544-55	5.4	39
75	Comparative study of the effectiveness and limitations of current methods for detecting sequence coevolution. *Bioinformatics*, **2015**, 31, 1929-37	7.2	17
74	Structure, Dynamics, and Allosteric Potential of Ionotropic Glutamate Receptor N-Terminal Domains. *Biophysical Journal*, **2015**, 109, 1136-48	2.9	21

73	Designing inhibitors of cytochrome c/cardiolipin peroxidase complexes: mitochondria-targeted imidazole-substituted fatty acids. *Free Radical Biology and Medicine*, **2014**, 71, 221-230	7.8	33
72	A genome-wide RNAi screen identifies potential drug targets in a C. elegans model of 1-antitrypsin deficiency. *Human Molecular Genetics*, **2014**, 23, 5123-32	5.6	37
71	Coupling between neurotransmitter translocation and protonation state of a titratable residue during Na +-coupled transport. *Biophysical Journal*, **2014**, 106, 2547-8	2.9	2
70	Evol and ProDy for bridging protein sequence evolution and structural dynamics. *Bioinformatics*, **2014**, 30, 2681-3	7.2	130
69	Significance of p53 dynamics in regulating apoptosis in response to ionizing radiation, and polypharmacological strategies. *Scientific Reports*, **2014**, 4, 6245	4.9	26
68	ATPase subdomain IA is a mediator of interdomain allostery in Hsp70 molecular chaperones. *PLoS Computational Biology*, **2014**, 10, e1003624	5	65
67	Exploring the conformational transitions of biomolecular systems using a simple two-state anisotropic network model. *PLoS Computational Biology*, **2014**, 10, e1003521	5	94
66	Complete mapping of substrate translocation highlights the role of LeuT N-terminal segment in regulating transport cycle. *PLoS Computational Biology*, **2014**, 10, e1003879	5	54
65	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	6	109
64	Global transitions of proteins explored by a multiscale hybrid methodology: application to adenylate kinase. *Biophysical Journal*, **2013**, 105, 1643-52	2.9	52
63	Predicting drug-target interactions using probabilistic matrix factorization. *Journal of Chemical Information and Modeling*, **2013**, 53, 3399-409	6.1	108
62	Cardiolipin externalization to the outer mitochondrial membrane acts as an elimination signal for mitophagy in neuronal cells. *Nature Cell Biology*, **2013**, 15, 1197-1205	23.4	597
61	Coupled global and local changes direct substrate translocation by neurotransmitter-sodium symporter ortholog LeuT. *Biophysical Journal*, **2013**, 105, 630-9	2.9	48
60	Intracellular gating in an inward-facing state of aspartate transporter Glt(Ph) is regulated by the movements of the helical hairpin HP2. *Journal of Biological Chemistry*, **2013**, 288, 8231-8237	5.4	36
59	Comparative dynamics of NMDA- and AMPA-glutamate receptor N-terminal domains. *Structure*, **2012**, 20, 1838-49	5.2	33
58	FlexE: Using elastic network models to compare models of protein structure. *Journal of Chemical Theory and Computation*, **2012**, 8, 3985-3991	6.4	19
57	Druggability Assessment of Allosteric Proteins by Dynamics Simulations in the Presence of Probe Molecules. *Journal of Chemical Theory and Computation*, **2012**, 8, 2435-2447	6.4	113
56	Constraints imposed by the membrane selectively guide the alternating access dynamics of the glutamate transporter GltPh. *Biophysical Journal*, **2012**, 102, 1331-40	2.9	38

55	The interface of protein structure, protein biophysics, and molecular evolution. *Protein Science*, **2012**, 21, 769-85	6.3	136
54	Sequence evolution correlates with structural dynamics. *Molecular Biology and Evolution*, **2012**, 29, 2253-63	8.9	105
53	A conformational switch in a partially unwound helix selectively determines the pathway for substrate release from the carnitine/γ-butyrobetaine antiporter CaiT. *Journal of Biological Chemistry*, **2012**, 287, 31823-32	5.4	16
52	ProDy: protein dynamics inferred from theory and experiments. *Bioinformatics*, **2011**, 27, 1575-7	7.2	626
51	Development of small-molecule PUMA inhibitors for mitigating radiation-induced cell death. *Current Topics in Medicinal Chemistry*, **2011**, 11, 281-90	3	49
50	Dynamics and allosteric potential of the AMPA receptor N-terminal domain. *EMBO Journal*, **2011**, 30, 972-82	13	50
49	Cooperative dynamics of proteins unraveled by network models. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 426-439	7.9	13
48	Pre-existing soft modes of motion uniquely defined by native contact topology facilitate ligand binding to proteins. *Protein Science*, **2011**, 20, 1645-58	6.3	74
47	The mechanism of substrate release by the aspartate transporter GltPh: insights from simulations. *Molecular BioSystems*, **2011**, 7, 832-42		41
46	Sodium-coupled Secondary Transporters: Insights from Structure-based Computations **2011**, 199-229		2
45	Protonation of glutamate 208 induces the release of agmatine in an outward-facing conformation of an arginine/agmatine antiporter. *Journal of Biological Chemistry*, **2011**, 286, 19693-701	5.4	17
44	Large collective motions regulate the functional properties of glutamate transporter trimers. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 15141-6	11.5	50
43	On the functional significance of soft modes predicted by coarse-grained models for membrane proteins. *Journal of General Physiology*, **2010**, 135, 563-73	3.4	43
42	On the conservation of the slow conformational dynamics within the amino acid kinase family: NAGK the paradigm. *PLoS Computational Biology*, **2010**, 6, e1000738	5	35
41	Global dynamics of proteins: bridging between structure and function. *Annual Review of Biophysics*, **2010**, 39, 23-42	21.1	454
40	Normal mode analysis of biomolecular structures: functional mechanisms of membrane proteins. *Chemical Reviews*, **2010**, 110, 1463-97	68.1	383
39	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, 14349-54	11.5	219
38	Molecular simulations elucidate the substrate translocation pathway in a glutamate transporter. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 2589-94	11.5	47

37	Allosteric transitions of supramolecular systems explored by network models: application to chaperonin GroEL. *PLoS Computational Biology*, **2009**, 5, e1000360	5	111
36	Principal component analysis of native ensembles of biomolecular structures (PCA_NEST): insights into functional dynamics. *Bioinformatics*, **2009**, 25, 606-14	7.2	101
35	Discovery of novel Myc-Max heterodimer disruptors with a three-dimensional pharmacophore model. *Journal of Medicinal Chemistry*, **2009**, 52, 1247-50	8.3	68
34	Elastic Network Models For Biomolecular Dynamics: Theory and Application to Membrane Proteins and Viruses. *World Scientific Lecture Notes in Complex Systems*, **2009**, 129-158		8
33	Mechanism of signal propagation upon retinal isomerization: insights from molecular dynamics simulations of rhodopsin restrained by normal modes. *Biophysical Journal*, **2008**, 95, 789-803	2.9	66
32	Toward a molecular understanding of the anisotropic response of proteins to external forces: insights from elastic network models. *Biophysical Journal*, **2008**, 94, 3424-35	2.9	70
31	Time-resolved mechanism of extracellular gate opening and substrate binding in a glutamate transporter. *Journal of Biological Chemistry*, **2008**, 283, 28680-90	5.4	82
30	Intrinsic dynamics of enzymes in the unbound state and relation to allosteric regulation. *Current Opinion in Structural Biology*, **2007**, 17, 633-40	8.1	253
29	Signal propagation in proteins and relation to equilibrium fluctuations. *PLoS Computational Biology*, **2007**, 3, 1716-26	5	171
28	Markov methods for hierarchical coarse-graining of large protein dynamics. *Journal of Computational Biology*, **2007**, 14, 765-76	1.7	20
27	Anisotropic network model: systematic evaluation and a new web interface. *Bioinformatics*, **2006**, 22, 2619-27	7.2	237
26	Common mechanism of pore opening shared by five different potassium channels. *Biophysical Journal*, **2006**, 90, 3929-40	2.9	79
25	Coupling between catalytic site and collective dynamics: a requirement for mechanochemical activity of enzymes. *Structure*, **2005**, 13, 893-904	5.2	225
24	Coarse-grained normal mode analysis in structural biology. *Current Opinion in Structural Biology*, **2005**, 15, 586-92	8.1	601
23	Structural changes involved in protein binding correlate with intrinsic motions of proteins in the unbound state. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 18908-13	11.5	313
22	Dynamics of large proteins through hierarchical levels of coarse-grained structures. *Journal of Computational Chemistry*, **2002**, 23, 119-27	3.5	207
21	Residue packing in proteins: Uniform distribution on a coarse-grained scale. *Journal of Chemical Physics*, **2002**, 116, 2269-2276	3.9	32
20	Functional motions of influenza virus hemagglutinin: a structure-based analytical approach. *Biophysical Journal*, **2002**, 82, 569-81	2.9	67

19	Transition states and the meaning of Phi-values in protein folding kinetics. *Nature Structural Biology*, **2001**, 8, 765-9		118
18	Dynamics of proteins predicted by molecular dynamics simulations and analytical approaches: Application to α-amylase inhibitor. *Proteins: Structure, Function and Bioinformatics*, **2000**, 40, 512-524	4.2	234
17	Dynamics of proteins predicted by molecular dynamics simulations and analytical approaches: Application to α-amylase inhibitor **2000**, 40, 512		5
16	Vibrational dynamics of transfer RNAs: comparison of the free and synthetase-bound forms. *Journal of Molecular Biology*, **1998**, 281, 871-84	6.5	116
15	Vibrational Dynamics of Folded Proteins: Significance of Slow and Fast Motions in Relation to Function and Stability. *Physical Review Letters*, **1998**, 80, 2733-2736	7.4	326
14	Gaussian Dynamics of Folded Proteins. *Physical Review Letters*, **1997**, 79, 3090-3093	7.4	582
13	Direct evaluation of thermal fluctuations in proteins using a single-parameter harmonic potential. *Folding & Design*, **1997**, 2, 173-81		1073
12	Relative Contributions of Coupled Rotations and Small-Amplitude Torsions to Conformational Relaxation in Polymers. *Macromolecules*, **1996**, 29, 8942-8947	5.5	8
11	Mechanisms of the Exchange of Diblock Copolymers between Micelles at Dynamic Equilibrium. *Macromolecules*, **1996**, 29, 4764-4771	5.5	79
10	Computer simulations of two-dimensional trifunctional bimodal networks. *Macromolecular Theory and Simulations*, **1994**, 3, 151-161	1.5	16
9	Orientational and conformational correlations in deformed polymer chains with fixed end-to-end separation: A Brownian dynamics simulation study. *Journal of Chemical Physics*, **1992**, 97, 4428-4437	3.9	8
8	Time-dependent probability distribution functions for orientational motions of segments in polymer chains. *Journal of Chemical Physics*, **1992**, 97, 4438-4444	3.9	2
7	Stochastic treatment of conformational transitions of polymer chains in the sub-Rouse regime. *Macromolecules*, **1991**, 24, 3618-3626	5.5	9
6	A closed form solution for the internal dynamics of polymer chains. I. Bonds with independent rotational potentials. *Journal of Chemical Physics*, **1990**, 92, 4513-4518	3.9	4
5	Anisotropy of static and dynamic orientational correlations in N-alkanes. *Journal of Chemical Physics*, **1988**, 88, 1228-1234	3.9	14
4	Effect of flow on solutions of rodlike molecules. *Journal of Polymer Science, Part B: Polymer Physics*, **1986**, 24, 1361-1371	2.6	8
3	Disulfide bridge formation prevents CaMKII/Calmodulin interaction in Parkinson's disease		1
2	Impact of South African 501.V2 Variant on SARS-CoV-2 Spike Infectivity and Neutralization: A Structure-based Computational Assessment		35

1 Dynamics of proteins predicted by molecular dynamics simulations and analytical approaches: Application to α-amylase inhibitor 2