Gennady M Verkhivker

List of Publications by Citations

135 papers	4,032 citations	35 h-index	59 g-index
161 ext. papers	4,697 ext. citations	4.7 avg, IF	6.19 L-index

#	Paper	IF	Citations
135	Molecular recognition of the inhibitor AG-1343 by HIV-1 protease: conformationally flexible docking by evolutionary programming. *Chemistry and Biology*, **1995**, 2, 317-24		564
134	Deciphering common failures in molecular docking of ligand-protein complexes. *Journal of Computer-Aided Molecular Design*, **2000**, 14, 731-51	4.2	168
133	MOIL: A program for simulations of macromolecules. *Computer Physics Communications*, **1995**, 91, 159-189	4.2	145
132	Energy landscape theory, funnels, specificity, and optimal criterion of biomolecular binding. *Physical Review Letters*, **2003**, 90, 188101	7.4	134
131	Empirical free energy calculations of ligand-protein crystallographic complexes. I. Knowledge-based ligand-protein interaction potentials applied to the prediction of human immunodeficiency virus 1 protease binding affinity. *Protein Engineering, Design and Selection*, **1995**, 8, 677-91	1.9	128
130	Modeling signal propagation mechanisms and ligand-based conformational dynamics of the Hsp90 molecular chaperone full-length dimer. *PLoS Computational Biology*, **2009**, 5, e1000323	5	125
129	Complexity and simplicity of ligand-macromolecule interactions: the energy landscape perspective. *Current Opinion in Structural Biology*, **2002**, 12, 197-203	8.1	99
128	Simulating disorder-order transitions in molecular recognition of unstructured proteins: where folding meets binding. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 5148-53	11.5	95
127	Elucidation of the Hsp90 C-terminal inhibitor binding site. *ACS Chemical Biology*, **2011**, 6, 800-7	4.9	84
126	Unraveling principles of lead discovery: from unfrustrated energy landscapes to novel molecular anchors. *Proceedings of the National Academy of Sciences of the United States of America*, **1996**, 93, 8945-50	11.5	82
125	Dynamics-Based Discovery of Allosteric Inhibitors: Selection of New Ligands for the C-terminal Domain of Hsp90. *Journal of Chemical Theory and Computation*, **2010**, 6, 2978-89	6.4	70
124	A systematic protocol for the characterization of Hsp90 modulators. *Bioorganic and Medicinal Chemistry*, **2011**, 19, 684-92	3.4	70
123	Cancer driver mutations in protein kinase genes. *Cancer Letters*, **2009**, 281, 117-27	9.9	65
122	Hierarchical modeling of activation mechanisms in the ABL and EGFR kinase domains: thermodynamic and mechanistic catalysts of kinase activation by cancer mutations. *PLoS Computational Biology*, **2009**, 5, e1000487	5	63
121	Computational modeling of allosteric communication reveals organizing principles of mutation-induced signaling in ABL and EGFR kinases. *PLoS Computational Biology*, **2011**, 7, e1002179	5	62
120	Computational Analysis of Residue Interaction Networks and Coevolutionary Relationships in the Hsp70 Chaperones: A Community-Hopping Model of Allosteric Regulation and Communication. *PLoS Computational Biology*, **2017**, 13, e1005299	5	62
119	Computational modeling of allosteric regulation in the hsp90 chaperones: a statistical ensemble analysis of protein structure networks and allosteric communications. *PLoS Computational Biology*, **2014**, 10, e1003679	5	61

118	Understanding ligand-based modulation of the Hsp90 molecular chaperone dynamics at atomic resolution. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 7976-81	11.5	60
117	On the exergy analysis of power plants. *Energy Conversion and Management*, **2001**, 42, 2053-2059	10.6	58
116	Sequence and structure signatures of cancer mutation hotspots in protein kinases. *PLoS ONE*, **2009**, 4, e7485	3.7	57
115	Predicting structural effects in HIV-1 protease mutant complexes with flexible ligand docking and protein side-chain optimization. *Proteins: Structure, Function and Bioinformatics*, **1998**, 33, 295-310	4.2	56
114	Computer simulations of ligand–protein binding with ensembles of protein conformations: A Monte Carlo study of HIV-1 protease binding energy landscapes. *International Journal of Quantum Chemistry*, **1999**, 72, 73-84	2.1	44
113	Locally enhanced sampling in free energy calculations: Application of mean field approximation to accurate calculation of free energy differences. *Journal of Chemical Physics*, **1992**, 97, 7838-7841	3.9	44
112	A mean field model of ligand-protein interactions: implications for the structural assessment of human immunodeficiency virus type 1 protease complexes and receptor-specific binding. *Proceedings of the National Academy of Sciences of the United States of America*, **1996**, 93, 60-4	11.5	43
111	Molecular Dynamics Simulations and Structural Network Analysis of c-Abl and c-Src Kinase Core Proteins: Capturing Allosteric Mechanisms and Communication Pathways from Residue Centrality. *Journal of Chemical Information and Modeling*, **2015**, 55, 1645-62	6.1	41
110	Quantifying intrinsic specificity: a potential complement to affinity in drug screening. *Physical Review Letters*, **2007**, 99, 198101	7.4	41
109	Integrated Computational Approaches and Tools forAllosteric Drug Discovery. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	41
108	The use of chemical recuperation of heat in a power plant. *Energy*, **2004**, 29, 379-388	7.9	40
107	Computational modeling of structurally conserved cancer mutations in the RET and MET kinases: the impact on protein structure, dynamics, and stability. *Biophysical Journal*, **2009**, 96, 858-74	2.9	39
106	Exploring the energy landscapes of molecular recognition by a genetic algorithm: Analysis of the requirements for robust docking of HIV-1 protease and FKBP-12 complexes. *Proteins: Structure, Function and Bioinformatics*, **1996**, 25, 342-353	4.2	39
105	Impact of Early Pandemic Stage Mutations on Molecular Dynamics of SARS-CoV-2 M. *Journal of Chemical Information and Modeling*, **2020**, 60, 5080-5102	6.1	38
104	Probing Allosteric Inhibition Mechanisms of the Hsp70 Chaperone Proteins Using Molecular Dynamics Simulations and Analysis of the Residue Interaction Networks. *Journal of Chemical Information and Modeling*, **2016**, 56, 1490-517	6.1	37
103	Dancing through Life: Molecular Dynamics Simulations and Network-Centric Modeling of Allosteric Mechanisms in Hsp70 and Hsp110 Chaperone Proteins. *PLoS ONE*, **2015**, 10, e0143752	3.7	37
102	Probing molecular mechanisms of the Hsp90 chaperone: biophysical modeling identifies key regulators of functional dynamics. *PLoS ONE*, **2012**, 7, e37605	3.7	37
101	Microscopic modeling of ligand diffusion through the protein leghemoglobin: computer simulations and experiments. *Journal of the American Chemical Society*, **1992**, 114, 7866-7878	16.4	36

100	Integration of network models and evolutionary analysis into high-throughput modeling of protein dynamics and allosteric regulation: theory, tools and applications. *Briefings in Bioinformatics*, **2020**, 21, 815-835	13.4	34
99	Dissecting Structure-Encoded Determinants of Allosteric Cross-Talk between Post-Translational Modification Sites in the Hsp90 Chaperones. *Scientific Reports*, **2018**, 8, 6899	4.9	32
98	Differential modulation of functional dynamics and allosteric interactions in the Hsp90-cochaperone complexes with p23 and Aha1: a computational study. *PLoS ONE*, **2013**, 8, e71936	3.7	32
97	Towards understanding the mechanisms of molecular recognition by computer simulations of ligand-protein interactions. *Journal of Molecular Recognition*, **1999**, 12, 371-89	2.6	32
96	Molecular Determinants Underlying Binding Specificities of the ABL Kinase Inhibitors: Combining Alanine Scanning of Binding Hot Spots with Network Analysis of Residue Interactions and Coevolution. *PLoS ONE*, **2015**, 10, e0130203	3.7	29
95	The energy landscape analysis of cancer mutations in protein kinases. *PLoS ONE*, **2011**, 6, e26071	3.7	29
94	Monte Carlo simulations of the peptide recognition at the consensus binding site of the constant fragment of human immunoglobulin G: the energy landscape analysis of a hot spot at the intermolecular interface. *Proteins: Structure, Function and Bioinformatics*, **2002**, 48, 539-57	4.2	29
93	Structure-based network analysis of activation mechanisms in the ErbB family of receptor tyrosine kinases: the regulatory spine residues are global mediators of structural stability and allosteric interactions. *PLoS ONE*, **2014**, 9, e113488	3.7	28
92	Atomistic Modeling of the ABL Kinase Regulation by Allosteric Modulators Using Structural Perturbation Analysis and Community-Based Network Reconstruction of Allosteric Communications. *Journal of Chemical Theory and Computation*, **2019**, 15, 3362-3380	6.4	27
91	Parallel simulated tempering dynamics of ligandProtein binding with ensembles of protein conformations. *Chemical Physics Letters*, **2001**, 337, 181-189	2.5	26
90	Allosteric regulation of the Hsp90 dynamics and stability by client recruiter cochaperones: protein structure network modeling. *PLoS ONE*, **2014**, 9, e86547	3.7	26
89	Molecular Simulations and Network Modeling Reveal an Allosteric Signaling in the SARS-CoV-2 Spike Proteins. *Journal of Proteome Research*, **2020**, 19, 4587-4608	5.6	26
88	Computational detection of the binding-site hot spot at the remodeled human growth hormone-receptor interface. *Proteins: Structure, Function and Bioinformatics*, **2003**, 53, 201-19	4.2	25
87	Structure-functional prediction and analysis of cancer mutation effects in protein kinases. *Computational and Mathematical Methods in Medicine*, **2014**, 2014, 653487	2.8	23
86	In silico profiling of tyrosine kinases binding specificity and drug resistance using Monte Carlo simulations with the ensembles of protein kinase crystal structures. *Biopolymers*, **2007**, 85, 333-48	2.2	23
85	Integrating ligand-based and protein-centric virtual screening of kinase inhibitors using ensembles of multiple protein kinase genes and conformations. *Journal of Chemical Information and Modeling*, **2012**, 52, 2501-15	6.1	22
84	Structural and computational biology of the molecular chaperone Hsp90: from understanding molecular mechanisms to computer-based inhibitor design. *Current Topics in Medicinal Chemistry*, **2009**, 9, 1369-85	3	22
83	Exploring Molecular Mechanisms of Paradoxical Activation in the BRAF Kinase Dimers: Atomistic Simulations of Conformational Dynamics and Modeling of Allosteric Communication Networks and Signaling Pathways. *PLoS ONE*, **2016**, 11, e0166583	3.7	22

82	Atomistic simulations and network-based modeling of the Hsp90-Cdc37 chaperone binding with Cdk4 client protein: A mechanism of chaperoning kinase clients by exploiting weak spots of intrinsically dynamic kinase domains. *PLoS ONE*, **2017**, 12, e0190267	3.7	22
81	Molecular dynamics simulations and modelling of the residue interaction networks in the BRAF kinase complexes with small molecule inhibitors: probing the allosteric effects of ligand-induced kinase dimerization and paradoxical activation. *Molecular BioSystems*, **2016**, 12, 3146-65		21
80	Biophysical simulations and structure-based modeling of residue interaction networks in the tumor suppressor proteins reveal functional role of cancer mutation hotspots in molecular communication. *Biochimica Et Biophysica Acta - General Subjects*, **2019**, 1863, 210-225	4	21
79	Integration of Random Forest Classifiers and Deep Convolutional Neural Networks for Classification and Biomolecular Modeling of Cancer Driver Mutations. *Frontiers in Molecular Biosciences*, **2019**, 6, 44	5.6	20
78	Experimentally guided structural modeling and dynamics analysis of Hsp90-p53 interactions: allosteric regulation of the Hsp90 chaperone by a client protein. *Journal of Chemical Information and Modeling*, **2013**, 53, 2962-78	6.1	20
77	Mean field analysis of FKBP12 complexes with FK506 and rapamycin: Implications for a role of crystallographic water molecules in molecular recognition and specificity. *Proteins: Structure, Function and Bioinformatics*, **1997**, 28, 313-324	4.2	20
76	Computational analysis of ligand binding dynamics at the intermolecular hot spots with the aid of simulated tempering and binding free energy calculations. *Journal of Molecular Graphics and Modelling*, **2004**, 22, 335-48	2.8	20
75	Exploring sequence-structure relationships in the tyrosine kinome space: functional classification of the binding specificity mechanisms for cancer therapeutics. *Bioinformatics*, **2007**, 23, 1919-26	7.2	19
74	Monte Carlo study of ligand–protein binding energy landscapes with the weighted histogram analysis method. *International Journal of Quantum Chemistry*, **1999**, 73, 113-121	2.1	18
73	Allosteric Regulation at the Crossroads of New Technologies: Multiscale Modeling, Networks, and Machine Learning. *Frontiers in Molecular Biosciences*, **2020**, 7, 136	5.6	18
72	Dynamic Network Modeling of Allosteric Interactions and Communication Pathways in the SARS-CoV-2 Spike Trimer Mutants: Differential Modulation of Conformational Landscapes and Signal Transmission via Cascades of Regulatory Switches. *Journal of Physical Chemistry B*, **2021**, 125, 850-873	3.4	18
71	Computational proteomics of biomolecular interactions in the sequence and structure space of the tyrosine kinome: deciphering the molecular basis of the kinase inhibitors selectivity. *Proteins: Structure, Function and Bioinformatics*, **2007**, 66, 912-29	4.2	17
70	Comparative Perturbation-Based Modeling of the SARS-CoV-2 Spike Protein Binding with Host Receptor and Neutralizing Antibodies: Structurally Adaptable Allosteric Communication Hotspots Define Spike Sites Targeted by Global Circulating Mutations. *Biochemistry*, **2021**, 60, 1459-1484	3.2	17
69	Integrated Biophysical Modeling of the SARS-CoV-2 Spike Protein Binding and Allosteric Interactions with Antibodies. *Journal of Physical Chemistry B*, **2021**, 125, 4596-4619	3.4	16
68	Dynamic View of Allosteric Regulation in the Hsp70 Chaperones by J-Domain Cochaperone and Post-Translational Modifications: Computational Analysis of Hsp70 Mechanisms by Exploring Conformational Landscapes and Residue Interaction Networks. *Journal of Chemical Information and Modeling*, **2020**, 60, 1614-1631	6.1	15
67	Functional Role and Hierarchy of the Intermolecular Interactions in Binding of Protein Kinase Clients to the Hsp90-Cdc37 Chaperone: Structure-Based Network Modeling of Allosteric Regulation. *Journal of Chemical Information and Modeling*, **2018**, 58, 405-421	6.1	15
66	Allosteric mechanism of the circadian protein Vivid resolved through Markov state model and machine learning analysis. *PLoS Computational Biology*, **2019**, 15, e1006801	5	15
65	Coevolution, Dynamics and Allostery Conspire in Shaping Cooperative Binding and Signal Transmission of the SARS-CoV-2 Spike Protein with Human Angiotensin-Converting Enzyme 2. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	14

64	Imprint of evolutionary conservation and protein structure variation on the binding function of protein tyrosine kinases. *Bioinformatics*, **2006**, 22, 1846-54	7.2	14
63	Protein conformational transitions coupled to binding in molecular recognition of unstructured proteins: deciphering the effect of intermolecular interactions on computational structure prediction of the p27Kip1 protein bound to the cyclin A-cyclin-dependent kinase 2 complex. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 796-16	4.2	14
62	Exploring the energy landscapes of molecular recognition by a genetic algorithm: analysis of the requirements for robust docking of HIV-1 protease and FKBP-12 complexes. *Proteins: Structure, Function and Bioinformatics*, **1996**, 25, 342-53	4.2	14
61	Machine Learning Classification and Structure-Functional Analysis of Cancer Mutations Reveal Unique Dynamic and Network Signatures of Driver Sites in Oncogenes and Tumor Suppressor Genes. *Journal of Chemical Information and Modeling*, **2018**, 58, 2131-2150	6.1	14
60	Ensemble-based modeling and rigidity decomposition of allosteric interaction networks and communication pathways in cyclin-dependent kinases: Differentiating kinase clients of the Hsp90-Cdc37 chaperone. *PLoS ONE*, **2017**, 12, e0186089	3.7	13
59	Hierarchy of simulation models in predicting structure and energetics of the Src SH2 domain binding to tyrosyl phosphopeptides. *Journal of Medicinal Chemistry*, **2002**, 45, 72-89	8.3	13
58	Simulating molecular mechanisms of the MDM2-mediated regulatory interactions: a conformational selection model of the MDM2 lid dynamics. *PLoS ONE*, **2012**, 7, e40897	3.7	13
57	Dynamics-based community analysis and perturbation response scanning of allosteric interaction networks in the TRAP1 chaperone structures dissect molecular linkage between conformational asymmetry and sequential ATP hydrolysis. *Biochimica Et Biophysica Acta - Proteins and Proteomics*,	4	13
56	Data-driven computational analysis of allosteric proteins by exploring protein dynamics, residue coevolution and residue interaction networks. *Biochimica Et Biophysica Acta - General Subjects*, **2019** ,	4	12
55	Hierarchy of simulation models in predicting molecular recognition mechanisms from the binding energy landscapes: structural analysis of the peptide complexes with SH2 domains. *Proteins: Structure, Function and Bioinformatics*, **2001**, 45, 456-70	4.2	12
54	Navigating ligand–protein binding free energy landscapes: universality and diversity of protein folding and molecular recognition mechanisms. *Chemical Physics Letters*, **2001**, 336, 495-503	2.5	10
53	Use of carbon dioxide as a heat carrier and working substance in atomic power stations. *Soviet Atomic Energy*, **1969**, 26, 430-432		10
52	Atomistic simulations of the HIV-1 protease folding inhibition. *Biophysical Journal*, **2008**, 95, 550-62	2.9	9
51	Design, Synthesis, and Evaluation of Dasatinib-Amino Acid and Dasatinib-Fatty Acid Conjugates as Protein Tyrosine Kinase Inhibitors. *ChemMedChem*, **2017**, 12, 86-99	3.7	8
50	Characterization of multiple stable conformers of the EC5 domain of E-cadherin and the interaction of EC5 with E-cadherin peptides. *Chemical Biology and Drug Design*, **2009**, 73, 584-98	2.9	8
49	Structural consensus in ligand-protein docking identifies recognition peptide motifs that bind streptavidin **1997**, 28, 421-433		8
48	Sequence recognition of alpha-LFA-1-derived peptides by ICAM-1 cell receptors: inhibitors of T-cell adhesion. *Chemical Biology and Drug Design*, **2007**, 70, 237-46	2.9	8
47	Structural modifications of ICAM-1 cyclic peptides to improve the activity to inhibit heterotypic adhesion of T cells. *Chemical Biology and Drug Design*, **2008**, 72, 27-33	2.9	8

46	Exploring Mechanisms of Communication Switching in the Hsp90-Cdc37 Regulatory Complexes with Client Kinases through Allosteric Coupling of Phosphorylation Sites: Perturbation-Based Modeling and Hierarchical Community Analysis of Residue Interaction Networks. *Journal of Chemical Theory and Computation*, **2020**, 16, 4706-4725	6.4	7
45	Comparative Dynamics and Functional Mechanisms of the CYP17A1 Tunnels Regulated by Ligand Binding. *Journal of Chemical Information and Modeling*, **2020**, 60, 3632-3647	6.1	7
44	Establishing Computational Approaches Towards Identifying Malarial Allosteric Modulators: A Case Study of Hsp70s. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	7
43	The role of covalent dimerization on the physical and chemical stability of the EC1 domain of human E-cadherin. *Journal of Pharmaceutical Sciences*, **2009**, 98, 3562-74	3.9	7
42	Examining ligand-protein interactions with binding-energy landscapes. *Theoretical Chemistry Accounts*, **1999**, 101, 138-142	1.9	7
41	Leveraging Structural Diversity and Allosteric Regulatory Mechanisms of Protein Kinases in the Discovery of Small Molecule Inhibitors. *Current Medicinal Chemistry*, **2017**, 24, 4838-4872	4.3	7
40	Interrogating Regulatory Mechanisms in Signaling Proteins by Allosteric Inhibitors and Activators: A Dynamic View Through the Lens of Residue Interaction Networks. *Advances in Experimental Medicine and Biology*, **2019**, 1163, 187-223	3.6	7
39	Dynamic Profiling of Binding and Allosteric Propensities of the SARS-CoV-2 Spike Protein with Different Classes of Antibodies: Mutational and Perturbation-Based Scanning Reveals the Allosteric Duality of Functionally Adaptable Hotspots. *Journal of Chemical Theory and Computation*, **2021**, 17, 4578-4598	6.4	7
38	Computational Modeling of the Hsp90 Interactions with Cochaperones and Small-Molecule Inhibitors. *Methods in Molecular Biology*, **2018**, 1709, 253-273	1.4	7
37	Allosteric Mechanism of the Hsp90 Chaperone Interactions with Cochaperones and Client Proteins by Modulating Communication Spines of Coupled Regulatory Switches: Integrative Atomistic Modeling of Hsp90 Signaling in Dynamic Interaction Networks. *Journal of Chemical Information and Modeling*, **2020**, 60, 3616-3631	6.1	6
36	Network-based modelling and percolation analysis of conformational dynamics and activation in the CDK2 and CDK4 proteins: dynamic and energetic polarization of the kinase lobes may determine divergence of the regulatory mechanisms. *Molecular BioSystems*, **2017**, 13, 2235-2253		6
35	Small-world networks of residue interactions in the Abl kinase complexes with cancer drugs: topology of allosteric communication pathways can determine drug resistance effects. *Molecular BioSystems*, **2015**, 11, 2082-95		6
34	Protein conformational transitions coupled to binding in molecular recognition of unstructured proteins: hierarchy of structural loss from all-atom Monte Carlo simulations of p27Kip1 unfolding-unbinding and structural determinants of the binding mechanism. *Biopolymers*, **2004**, 75, 420-33	2.2	6
33	Conformational Composition of 5-Alkyl-1,3-Oxathianes. *Russian Journal of General Chemistry*, **2001**, 71, 1487-1490	0.7	6
32	New trends in computational structure prediction of ligand-protein complexes for receptor-based drug design **1997**, 451-465		5
31	Structural bioinformatics and protein docking analysis of the molecular chaperone-kinase interactions: towards allosteric inhibition of protein kinases by targeting the hsp90-cdc37 chaperone machinery. *Pharmaceuticals*, **2013**, 6, 1407-28	5.2	4
30	Computational Studies of Allosteric Regulation in the Hsp90 Molecular Chaperone: From Functional Dynamics and Protein Structure Networks to Allosteric Communications and Targeted Anti-Cancer Modulators. *Israel Journal of Chemistry*, **2014**, 54, 1052-1064	3.4	3
29	Thermodynamic properties of uranium hexafluoride (UF6). *Soviet Atomic Energy*, **1968**, 24, 191-195		3

28	Impact of emerging mutations on the dynamic properties the SARS-CoV-2 main protease: an in silico investigation		3
27	Landscape-Based Mutational Sensitivity Cartography and Network Community Analysis of the SARS-CoV-2 Spike Protein Structures: Quantifying Functional Effects of the Circulating D614G Variant. *ACS Omega*, **2021**, 6, 16216-16233	3.9	3
26	Computational analysis of protein stability and allosteric interaction networks in distinct conformational forms of the SARS-CoV-2 spike D614G mutant: reconciling functional mechanisms through allosteric model of spike regulation. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-18	3.6	3
25	Making the invisible visible: Toward structural characterization of allosteric states, interaction networks, and allosteric regulatory mechanisms in protein kinases. *Current Opinion in Structural Biology*, **2021**, 71, 71-78	8.1	3
24	Mean field analysis of FKBP12 complexes with FK506 and rapamycin: implications for a role of crystallographic water molecules in molecular recognition and specificity. *Proteins: Structure, Function and Bioinformatics*, **1997**, 28, 313-24	4.2	3
23	Monte Carlo simulations of HIV-1 protease binding dynamics and thermodynamics with ensembles of protein conformations: Incorporating protein flexibility in deciphering mechanisms of molecular recognition. *Theoretical and Computational Chemistry*, **2001**, 289-340		2
22	Dissecting Molecular Principles of the Hsp90 Chaperone Regulation by Allosteric Modulators Using a Hierarchical Simulation Approach and Network Modeling of Allosteric Interactions: Conformational Selection Dictates the Diversity of Protein Responses and Ligand-Specific Functional Mechanisms. *Journal of Chemical Theory and Computation*, **2020**, 16, 6656-6677	6.4	2
21	Dimeric allostery mechanism of the plant circadian clock photoreceptor ZEITLUPE. *PLoS Computational Biology*, **2021**, 17, e1009168	5	2
20	Atomistic Simulations and In Silico Mutational Profiling of Protein Stability and Binding in the SARS-CoV-2 Spike Protein Complexes with Nanobodies: Molecular Determinants of Mutational Escape Mechanisms. *ACS Omega*, **2021**, 6, 26354-26371	3.9	2
19	Allosteric Control of Structural Mimicry and Mutational Escape in the SARS-CoV-2 Spike Protein Complexes with the ACE2 Decoys and Miniprotein Inhibitors: A Network-Based Approach for Mutational Profiling of Binding and Signaling. *Journal of Chemical Information and Modeling*, **2021**, 61, 5178-5191	6.1	2
18	Computational Analysis of Protein Stability and Allosteric Interaction Networks in Distinct Conformational Forms of the SARS-CoV-2 Spike D614G Mutant: Reconciling Functional Mechanisms through Allosteric Model of Spike Regulation		2
17	Exploring Mechanisms of Allosteric Regulation and Communication Switching in the Multiprotein Regulatory Complexes of the Hsp90 Chaperone with Cochaperones and Client Proteins: Atomistic Insights from Integrative Biophysical Modeling and Network Analysis of Conformational Landscapes. *Journal of Molecular Biology*, **2022**, 167506	6.5	2
16	Contribution from the aqueous phase to stability of Cs+ and Na+ cryptand[2.2.2] complexes. *Theoretical and Experimental Chemistry*, **1989**, 25, 697-698	1.3	1
15	Moil: A Molecular Dynamics Program with Emphasis on Conformational Searches and Reaction Path Calculations. *NATO ASI Series Series B: Physics*, **1994**, 165-191		1
14	Coarse-Grained Modeling of the HIV1 Protease Binding Mechanisms: II. Folding Inhibition. *Lecture Notes in Computer Science*, **2009**, 13-24	0.9	1
13	Comparative Perturbation-Based Modeling of the SARS-CoV-2 Spike Protein Binding with Host Receptor and Neutralizing Antibodies : Structurally Adaptable Allosteric Communication Hotspots Define Spike Sites Targeted by Global Circulating Mutations		1
12	Structural consensus in ligand-protein docking identifies recognition peptide motifs that bind streptavidin. *Proteins: Structure, Function and Bioinformatics*, **1997**, 28, 421-33	4.2	1
11	INTEGRATING GENETIC AND STRUCTURAL DATA ON HUMAN PROTEIN KINOME IN NETWORK-BASED MODELING OF KINASE SENSITIVITIES AND RESISTANCE TO TARGETED AND PERSONALIZED ANTICANCER DRUGS. *Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing*, **2016**, 21, 45-56	1.3	1

10	Computational proteomics analysis of binding mechanisms and molecular signatures of the HIV-1 protease drugs. *Artificial Intelligence in Medicine*, **2009**, 45, 197-206	7.4	0
9	Dissecting mutational allosteric effects in alkaline phosphatases associated with different Hypophosphatasia phenotypes: An integrative computational investigation.. *PLoS Computational Biology*, **2022**, 18, e1010009	5	0
8	Computational Detection of the Binding Site Hot Spot and Predicting Energetics of Ligand Binding at the Remodeled Human Growth Hormone-Receptor Interface Using a Hierarchy of Molecular Docking and Binding Free Energy Approaches **2005**, 231-271		
7	A Microscopic Study of Disorder-Order Transitions in Molecular Recognition of Unstructured Proteins: Hierarchy of Structural Loss and the Transition State Determination from Monte Carlo Simulations of P27KIP1 Protein Coupled Unfolding and Unbinding **2005**, 199-230		
6	A possible approach to determination of the preferred conformations in substituted saturated seven-membered rings. *Journal of Structural Chemistry*, **1986**, 26, 494-498	0.9	
5	Method for comparing nuclear power and production process installations. *Soviet Atomic Energy*, **1981**, 50, 350-353		
4	The predominant conformation of 1,3-dioxepane. *Theoretical and Experimental Chemistry*, **1981**, 17, 87-91	1.3	
3	A procedure for comparing various atomic electric power plant systems. *Soviet Atomic Energy*, **1973**, 34, 364-366		
2	Computational Proteomics of Biomolecular Interactions in Sequence and Structure Space of the Tyrosine Kinome: Evolutionary Constraints and Protein Conformational Selection Determine Binding Signatures of Cancer Drugs. *Lecture Notes in Computer Science*, **2007**, 604-611	0.9	
1	Coarse-Grained Modeling of the HIV1 Protease Binding Mechanisms: I. Targeting Structural Flexibility of the Protease Flaps and Implications for Drug Design. *Lecture Notes in Computer Science*, **2009**, 1-12	0.9	