Gennady M Verkhivker

List of Publications by Year
in descending order

143 papers	5,150 citations	81839 39 h-index	110317 64 g-index
161 all docs	161 docs citations	161 times ranked	4351 citing authors

#	Article	IF	Citations
1	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, 2022, 40, 9724-9741.	2.0	11
2	Conformational Flexibility and Local Frustration in the Functional States of the SARS-CoV-2 Spike B.1.1.7 and B.1.351 Variants: Mutation-Induced Allosteric Modulation Mechanism of Functional Dynamics and Protein Stability. International Journal of Molecular Sciences, 2022, 23, 1646.	1.8	2
3	Allosteric Determinants of the SARS-CoV-2 Spike Protein Binding with Nanobodies: Examining Mechanisms of Mutational Escape and Sensitivity of the Omicron Variant. International Journal of Molecular Sciences, 2022, 23, 2172.	1.8	5
4	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, 434, 167506.	2.0	9
5	Structural and Computational Studies of the SARS-CoV-2 Spike Protein Binding Mechanisms with Nanobodies: From Structure and Dynamics to Avidity-Driven Nanobody Engineering. International Journal of Molecular Sciences, 2022, 23, 2928.	1.8	8
6	Dissecting mutational allosteric effects in alkaline phosphatases associated with different Hypophosphatasia phenotypes: An integrative computational investigation. PLoS Computational Biology, 2022, 18, e1010009.	1.5	3
7	Landscape-Based Protein Stability Analysis and Network Modeling of Multiple Conformational States of the SARS-CoV-2 Spike D614G Mutant: Conformational Plasticity and Frustration-Induced Allostery as Energetic Drivers of Highly Transmissible Spike Variants. Journal of Chemical Information and Modeling, 2022, 62, 1956-1978.	2.5	5
8	Computer Simulations and Network-Based Profiling of Binding and Allosteric Interactions of SARS-CoV-2 Spike Variant Complexes and the Host Receptor: Dissecting the Mechanistic Effects of the Delta and Omicron Mutations. International Journal of Molecular Sciences, 2022, 23, 4376.	1.8	16
9	Biophysical Insight into the SARS-CoV2 Spikeâ€“ACE2 Interaction and Its Modulation by Hepcidin through a Multifaceted Computational Approach. ACS Omega, 2022, 7, 17024-17042.	1.6	9
10	Integrating Conformational Dynamics and Perturbation-Based Network Modeling for Mutational Profiling of Binding and Allostery in the SARS-CoV-2 Spike Variant Complexes with Antibodies: Balancing Local and Global Determinants of Mutational Escape Mechanisms. Biomolecules, 2022, 12, 964.	1.8	0
11	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.	1.2	60
12	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.	1.2	62
13	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.	1.6	10
14	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.	2.3	39
15	Dimeric allostery mechanism of the plant circadian clock photoreceptor ZEITLUPE. PLoS Computational Biology, 2021, 17, e1009168.	1.5	3
16	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.	1.6	11
17	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, 5172-5191.	2.5	26
18	Making the invisible visible: TowardÂstructural characterization of allosteric states, interaction networks, and allosteric regulatory mechanisms in protein kinases. Current Opinion in Structural Biology, 2021, 71, 71-78.	2.6	13

#	Article	IF	Citations
19	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.	1.2	66
20	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.	3.2	58
21	Molecular Simulations and Network Modeling Reveal an Allosteric Signaling in the SARS-CoV-2 Spike Proteins. Journal of Proteome Research, 2020, 19, 4587-4608.	1.8	72
22	Allosteric Regulation at the Crossroads of New Technologies: Multiscale Modeling, Networks, and Machine Learning. Frontiers in Molecular Biosciences, 2020, 7, 136.	1.6	44
23	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.	2.3	3
24	Impact of Early Pandemic Stage Mutations on Molecular Dynamics of SARS-CoV-2 M^{pro}. Journal of Chemical Information and Modeling, 2020, 60, 5080-5102.	2.5	62
25	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, 8268.	1.8	37
26	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.	2.3	15
27	Comparative Dynamics and Functional Mechanisms of the CYP17A1 Tunnels Regulated by Ligand Binding. Journal of Chemical Information and Modeling, 2020, 60, 3632-3647.	2.5	17
28	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.	2.5	10
29	Computational Modeling and Engineering of Allosteric Regulatory Mechanisms in Signaling Proteins: Integration of Multiscale Simulations, Network Biology and Machine Learning. Biophysical Journal, 2020, 118, 206a.	0.2	0
30	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.	2.5	27
31	Integrated Computational Approaches and Tools for Allosteric Drug Discovery. International Journal of Molecular Sciences, 2020, 21, 847.	1.8	73
32	Data-driven computational analysis of allosteric proteins by exploring protein dynamics, residue coevolution and residue interaction networks. Biochimica Et Biophysica Acta - General Subjects, 2019, , .	1.1	17
33	Establishing Computational Approaches Towards Identifying Malarial Allosteric Modulators: A Case Study of Plasmodium falciparum Hsp70s. International Journal of Molecular Sciences, 2019, 20, 5574.	1.8	12
34	Editorial: Machine Learning in Biomolecular Simulations. Frontiers in Molecular Biosciences, 2019, 6, 76.	1.6	4
35	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.	1.6	51
36	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.	2.3	46

#	Article	IF	Citations
37	Allosteric mechanism of the circadian protein Vivid resolved through Markov state model and machine learning analysis. PLoS Computational Biology, 2019, 15, e1006801.	1.5	19
38	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.	1.1	24
39	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.	0.8	17
40	Functional Role and Hierarchy of the Intermolecular Interactions in Binding of Protein Kinase Clients to the Hsp90â€“Cdc37 Chaperone: Structure-Based Network Modeling of Allosteric Regulation. Journal of Chemical Information and Modeling, 2018, 58, 405-421.	2.5	19
41	Computational Modeling of the Hsp90 Interactions with Cochaperones and Small-Molecule Inhibitors. Methods in Molecular Biology, 2018, 1709, 253-273.	0.4	7
42	Machine Learning Classification and Structureâ€“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.	2.5	20
43	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, 2018, 1866, 899-912.	1.1	16
44	Dissecting Structure-Encoded Determinants of Allosteric Cross-Talk between Post-Translational Modification Sites in the Hsp90 Chaperones. Scientific Reports, 2018, 8, 6899.	1.6	42
45	Leveraging Structural Diversity and Allosteric Regulatory Mechanisms of Protein Kinases in the Discovery of Small Molecule Inhibitors. Current Medicinal Chemistry, 2018, 24, 4838-4872.	1.2	9
46	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.	2.9	7
47	Design, Synthesis, and Evaluation of Dasatinibâ€“Amino Acid and Dasatinibâ€“Fatty Acid Conjugates as Protein Tyrosine Kinase Inhibitors. ChemMedChem, 2017, 12, 86-99.	1.6	11
48	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.	1.1	17
49	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.	1.5	91
50	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.	1.1	32
51	INTEGRATING GENETIC AND STRUCTURAL DATA ON HUMAN PROTEIN KINOME IN NETWORK-BASED MODELING OF KINASE SENSITIVITIES AND RESISTANCE TO TARGETED AND PERSONALIZED ANTICANCER DRUGS. , 2016, , .		1
52	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, 3146-3165.	2.9	25
53	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, 1490-1517.	2.5	42
54	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.	1.1	28

#	Article	IF	Citations
55	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.	0.7	1
56	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.	1.1	36
57	Dancing through Life: Molecular Dynamics Simulations and Network-Centric Modeling of Allosteric Mechanisms in Hsp70 and Hsp110 Chaperone Proteins. PLoS ONE, 2015, 10, e0143752.	1.1	45
58	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, 2082-2095.	2.9	6
59	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, 1645-1662.	2.5	52
60	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.	1.1	33
61	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.	1.5	77
62	Computational Studies of Allosteric Regulation in the Hsp90 Molecular Chaperone: From Functional Dynamics and Protein Structure Networks to Allosteric Communications and Targeted Antiâ€Cancer Modulators. Israel Journal of Chemistry, 2014, 54, 1052-1064.	1.0	5
63	Structure-Functional Prediction and Analysis of Cancer Mutation Effects in Protein Kinases. Computational and Mathematical Methods in Medicine, 2014, 2014, 1-24.	0.7	30
64	Allosteric Regulation of the Hsp90 Dynamics and Stability by Client Recruiter Cochaperones: Protein Structure Network Modeling. PLoS ONE, 2014, 9, e86547.	1.1	37
65	Experimentally Guided Structural Modeling and Dynamics Analysis of Hsp90â€“p53 Interactions: Allosteric Regulation of the Hsp90 Chaperone by a Client Protein. Journal of Chemical Information and Modeling, 2013, 53, 2962-2978.	2.5	25
66	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, 1407-1428.	1.7	7
67	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.	1.1	39
68	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, 2501-2515.	2.5	26
69	Probing Molecular Mechanisms of the Hsp90 Chaperone: Biophysical Modeling Identifies Key Regulators of Functional Dynamics. PLoS ONE, 2012, 7, e37605.	1.1	48
70	Simulating Molecular Mechanisms of the MDM2-Mediated Regulatory Interactions: A Conformational Selection Model of the MDM2 Lid Dynamics. PLoS ONE, 2012, 7, e40897.	1.1	13
71	Elucidation of the Hsp90 C-Terminal Inhibitor Binding Site. ACS Chemical Biology, 2011, 6, 800-807.	1.6	96
72	The Energy Landscape Analysis of Cancer Mutations in Protein Kinases. PLoS ONE, 2011, 6, e26071.	1.1	39

#	Article	IF	Citations
73	A systematic protocol for the characterization of Hsp90 modulators. Bioorganic and Medicinal Chemistry, 2011, 19, 684-692.	1.4	80
74	Computational Modeling of Allosteric Communication Reveals Organizing Principles of Mutation-Induced Signaling in ABL and EGFR Kinases. PLoS Computational Biology, 2011, 7, e1002179.	1.5	67
75	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, 2978-2989.	2.3	83
76	Sequence and Structure Signatures of Cancer Mutation Hotspots in Protein Kinases. PLoS ONE, 2009, 4, e7485.	1.1	66
77	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, 1369-1385.	1.0	24
78	Modeling Signal Propagation Mechanisms and Ligand-Based Conformational Dynamics of the Hsp90 Molecular Chaperone Full-Length Dimer. PLoS Computational Biology, 2009, 5, e1000323.	1.5	138
79	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.	1.5	65
80	Computational proteomics analysis of binding mechanisms and molecular signatures of the HIV-1 protease drugs. Artificial Intelligence in Medicine, 2009, 45, 197-206.	3.8	2
81	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, 3562-3574.	1.6	11
82	Characterization of Multiple Stable Conformers of the EC5 Domain of Eâ€cadherin and the Interaction of EC5 with Eâ€cadherin Peptides. Chemical Biology and Drug Design, 2009, 73, 584-598.	1.5	11
83	Cancer driver mutations in protein kinase genes. Cancer Letters, 2009, 281, 117-127.	3.2	84
84	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, 858-874.	0.2	40
85	Coarse-Grained Modeling of the HIVâ€“1 Protease Binding Mechanisms: II. Folding Inhibition. Lecture Notes in Computer Science, 2009, , 13-24.	1.0	1
86	Coarse-Grained Modeling of the HIVâ€“1 Protease Binding Mechanisms: I. Targeting Structural Flexibility of the Protease Flaps and Implications for Drug Design. Lecture Notes in Computer Science, 2009, , 1-12.	1.0	0
87	Structural Modifications of ICAMâ€1 Cyclic Peptides to Improve the Activity to Inhibit Heterotypic Adhesion of T cells. Chemical Biology and Drug Design, 2008, 72, 27-33.	1.5	10
88	Atomistic Simulations of the HIV-1 Protease Folding Inhibition. Biophysical Journal, 2008, 95, 550-562.	0.2	12
89	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, 7976-7981.	3.3	73
90	Exploring sequence-structure relationships in the tyrosine kinome space: functional classification of the binding specificity mechanisms for cancer therapeutics. Bioinformatics, 2007, 23, 1919-1926.	1.8	19

#	Article	IF	Citations
91	Quantifying Intrinsic Specificity: A Potential Complement to Affinity in Drug Screening. Physical Review Letters, 2007, 99, 198101.	2.9	46
92	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, 333-348.	1.2	25
93	Sequence Recognition of Î±â€ŁFAâ€‹â€derived Peptides by ICAMâ€‹ Cell Receptors: Inhibitors of Tâ€cell Adhesion. Chemical Biology and Drug Design, 2007, 70, 237-246.	1.5	14
94	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, 2006, 66, 912-929.	1.5	18
95	Imprint of evolutionary conservation and protein structure variation on the binding function of protein tyrosine kinases. Bioinformatics, 2006, 22, 1846-1854.	1.8	14
96	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.		0
97	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.		0
98	The use of chemical recuperation of heat in a power plant. Energy, 2004, 29, 379-388.	4.5	52
99	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-depend. Proteins: Structure, Function and Bioinformatics, 2004, 58, 706-716.	1.5	15
100	Protein conformational transitions coupled to binding in molecular recognition of unstructured proteins: Hierarchy of structural loss from all-atom Monte Carlo simulations ofp27Kip1 unfolding-unbinding and structural determinants of the binding mechanism. Biopolymers, 2004, 75, 420-433.	1.2	7
101	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, 335-348.	1.3	23
102	Computational detection of the binding-site hot spot at the remodeled human growth hormone-receptor interface. Proteins: Structure, Function and Bioinformatics, 2003, 53, 201-219.	1.5	27
103	Energy Landscape Theory, Funnels, Specificity, and Optimal Criterion of Biomolecular Binding. Physical Review Letters, 2003, 90, 188101.	2.9	145
104	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, 5148-5153.	3.3	102
105	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.	2.9	13
106	Complexity and simplicity of ligandâ€“macromolecule interactions: the energy landscape perspective. Current Opinion in Structural Biology, 2002, 12, 197-203.	2.6	106
107	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, 539-557.	1.5	30
108	Zero-emissions gas-fired cogeneration of power and hydrogen. International Journal of Hydrogen Energy, 2001, 26, 1109-1113.	3.8	1

#	Article	IF	Citations
109	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, 456-470.	1.5	12
110	Navigating ligandâ€“protein binding free energy landscapes: universality and diversity of protein folding and molecular recognition mechanisms. Chemical Physics Letters, 2001, 336, 495-503.	1.2	11
111	Parallel simulated tempering dynamics of ligandâ€“protein binding with ensembles of protein conformations. Chemical Physics Letters, 2001, 337, 181-189.	1.2	26
112	Conformational Composition of 5-Alkyl-1,3-Oxathianes. Russian Journal of General Chemistry, 2001, 71, 1487-1490.	0.3	7
113	On the exergy analysis of power plants. Energy Conversion and Management, 2001, 42, 2053-2059.	4.4	65
114	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.	0.2	2
115	Deciphering common failures in molecular docking of ligand-protein complexes. Journal of Computer-Aided Molecular Design, 2000, 14, 731-751.	1.3	192
116	Examining ligand-protein interactions with binding-energy landscapes. Theoretical Chemistry Accounts, 1999, 101, 138-142.	0.5	10
117	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.	1.0	52
118	Monte Carlo study of ligand-protein binding energy landscapes with the weighted histogram analysis method. International Journal of Quantum Chemistry, 1999, 73, 113-121.	1.0	19
119	Towards understanding the mechanisms of molecular recognition by computer simulations of ligand-protein interactions. , 1999, 12, 371-389.		37
120	Predicting structural effects in HIV-1 protease mutant complexes with flexible ligand docking and protein side-chain optimization. , 1998, 33, 295-310.		64
121	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.	1.5	21
122	Structural consensus in ligand-protein docking identifies recognition peptide motifs that bind streptavidin. , 1997, 28, 421-433.		10
123	New trends in computational structure prediction of ligand-protein complexes for receptor-based drug design. , 1997, , 451-465.		5
124	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.	1.5	4
125	Structural consensus in ligand-protein docking identifies recognition peptide motifs that bind streptavidin. Proteins: Structure, Function and Bioinformatics, 1997, 28, 421-33.	1.5	1
126	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, 60-64.	3.3	44

#	Article	IF	Citations
127	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, 8945-8950.	3.3	86
128	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.	1.5	19
129	Exploring the energy landscapes of molecular recognition by a genetic algorithm: Analysis of the requirements for robust docking of HIVâ€1 protease and FKBPâ€12 complexes. Proteins: Structure, Function and Bioinformatics, 1996, 25, 342-353.	1.5	44
130	MOIL: A program for simulations of macromolecules. Computer Physics Communications, 1995, 91, 159-189.	3.0	154
131	Molecular recognition of the inhibitor AG-1343 by HIV-1 protease: conformationally flexible docking by evolutionary programming. Chemistry and Biology, 1995, 2, 317-324.	6.2	622
132	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, 677-691.	1.0	140
133	Moil: A Molecular Dynamics Program with Emphasis on Conformational Searches and Reaction Path Calculations. NATO ASI Series Series B: Physics, 1994, , 165-191.	0.2	2
134	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.	1.2	47
135	Microscopic modeling of ligand diffusion through the protein leghemoglobin: computer simulations and experiments. Journal of the American Chemical Society, 1992, 114, 7866-7878.	6.6	37
136	Contribution from the aqueous phase to stability of Cs+ and Na+ cryptand[2.2.2] complexes. Theoretical and Experimental Chemistry, 1989, 25, 697-698.	0.2	1
137	A possible approach to determination of the preferred conformations in substituted saturated seven-membered rings. Journal of Structural Chemistry, 1986, 26, 494-498.	0.3	0
138	Method for comparing nuclear power and production process installations. Soviet Atomic Energy, 1981, 50, 350-353.	0.1	0
139	The predominant conformation of 1,3-dioxepane. Theoretical and Experimental Chemistry, 1981, 17, 87-91.	0.2	0
140	A procedure for comparing various atomic electric power plant systems. Soviet Atomic Energy, 1973, 34, 364-366.	0.1	0
141	Use of carbon dioxide as a heat carrier and working substance in atomic power stations. Soviet Atomic Energy, 1969, 26, 430-432.	0.1	14
142	Thermodynamic properties of uranium hexafluoride (UF6). Soviet Atomic Energy, 1968, 24, 191-195.	0.1	6
143	Frustration-driven allosteric regulation and signal transmission in the SARS-CoV-2 spike omicron trimer structures: a crosstalk of the omicron mutation sites allosterically regulates tradeoffs of protein stability and conformational adaptability. Physical Chemistry Chemical Physics, 0, , .	1.3	9