

# Haruki Nakamura

## List of Publications by Year in descending order

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157  
papers

12,394  
citations

36203

51  
h-index

27345

106  
g-index

164  
all docs

164  
docs citations

164  
times ranked

12326  
citing authors

#	ARTICLE	IF	CITATIONS
1	Difference of binding modes among three ligands to a receptor mSin3B corresponding to their inhibitory activities. <i>Scientific Reports</i> , 2021, 11, 6178.	1.6	10
2	Announcing changes to the publishing procedures of “Biophysics and Physicobiology” (BPPB) the Biophysical Society of Japan’s English language biophysics journal. <i>Biophysical Reviews</i> , 2021, 13, 813-814.	1.5	2
3	Molecular Interaction Mechanism of a 14-3-3 Protein with a Phosphorylated Peptide Elucidated by Enhanced Conformational Sampling. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4867-4880.	2.5	13
4	Big data science at AMED-BINDS. <i>Biophysical Reviews</i> , 2020, 12, 221-224.	1.5	5
5	Editorial for the Special Issue of <i>Biophysical Reviews</i> focused on the Biophysical Society of Japan with select scientific content from the 57th BSJ annual meeting, Miyazaki, Japan. <i>Biophysical Reviews</i> , 2020, 12, 183-185.	1.5	11
6	How A Novel Scientific Concept Was Coined the “Molten Globule State”. <i>Biomolecules</i> , 2020, 10, 269.	1.8	13
7	myPresto/omegagene 2020: a molecular dynamics simulation engine for virtual-system coupled sampling. <i>Biophysics and Physicobiology</i> , 2020, 17, 140-146.	0.5	8
8	The Papers that Influenced My Career: Creamer and Rose. <i>Seibutsu Butsuri</i> , 2020, 60, 190-191.	0.0	0
9	Multidimensional virtual-system coupled canonical molecular dynamics to compute free-energy landscapes of peptide multimer assembly. <i>Journal of Computational Chemistry</i> , 2019, 40, 2453-2463.	1.5	14
10	Free-energy landscape of molecular interactions between endothelin 1 and human endothelin type B receptor: fly-casting mechanism. <i>Protein Engineering, Design and Selection</i> , 2019, 32, 297-308.	1.0	15
11	Hydrogen bond donors and acceptors are generally depolarized in $\alpha$ -helices as revealed by a molecular tailoring approach. <i>Journal of Computational Chemistry</i> , 2019, 40, 2043-2052.	1.5	9
12	Multimodal Structural Distribution of the p53 C-Terminal Domain upon Binding to S100B via a Generalized Ensemble Method: From Disorder to Extradisorder. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2597-2607.	2.3	14
13	Protein Data Bank: the single global archive for 3D macromolecular structure data. <i>Nucleic Acids Research</i> , 2019, 47, D520-D528.	6.5	671
14	Molecular dynamics coupled with a virtual system for effective conformational sampling. <i>Journal of Computational Chemistry</i> , 2018, 39, 1291-1299.	1.5	5
15	Phosphorylation of an intrinsically disordered region of Ets1 shifts a multi-modal interaction ensemble to an auto-inhibitory state. <i>Nucleic Acids Research</i> , 2018, 46, 2243-2251.	6.5	34
16	Foreword to “Multiscale structural biology: biophysical principles and mechanisms underlying the action of bio-nanomachines”, a special issue in Honour of Fumio Arisaka’s 70th birthday. <i>Biophysical Reviews</i> , 2018, 10, 105-129.	1.5	4
17	Data Science and PDBj Activities. <i>Seibutsu Butsuri</i> , 2018, 58, 071-077.	0.0	0
18	New tools and functions in data-out activities at Protein Data Bank Japan (PDBj). <i>Protein Science</i> , 2018, 27, 95-102.	3.1	90

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19	Overall Introduction and Rationale, with View from Computational Biology. <i>Advances in Experimental Medicine and Biology</i> , 2018, 1105, 3-9.	0.8	1
20	Worldwide Protein Data Bank biocuration supporting open access to high-quality 3D structural biology data. <i>Database: the Journal of Biological Databases and Curation</i> , 2018, 2018, .	1.4	45
21	OneDep: Unified wwPDB System for Deposition, Biocuration, and Validation of Macromolecular Structures in the PDB Archive. <i>Structure</i> , 2017, 25, 536-545.	1.6	130
22	Accurate Prediction of Complex Structure and Affinity for a Flexible Protein Receptor and Its Inhibitor. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2389-2399.	2.3	43
23	Protein Data Bank (PDB): The Single Global Macromolecular Structure Archive. <i>Methods in Molecular Biology</i> , 2017, 1607, 627-641.	0.4	592
24	PDB-Dev: a Prototype System for Depositing Integrative/Hybrid Structural Models. <i>Structure</i> , 2017, 25, 1317-1318.	1.6	84
25	Validation of Structures in the Protein Data Bank. <i>Structure</i> , 2017, 25, 1916-1927.	1.6	210
26	Protein Data Bank Japan (PDBj): updated user interfaces, resource description framework, analysis tools for large structures. <i>Nucleic Acids Research</i> , 2017, 45, D282-D288.	6.5	108
27	Enhancement of canonical sampling by virtual-state transitions. <i>Journal of Chemical Physics</i> , 2017, 146, 044104.	1.2	12
28	Multi-dimensional virtual system introduced to enhance canonical sampling. <i>Journal of Chemical Physics</i> , 2017, 147, 134102.	1.2	8
29	Molmil: a molecular viewer for the PDB and beyond. <i>Journal of Cheminformatics</i> , 2016, 8, 42.	2.8	56
30	A critical appraisal of the zero-multipole method: Structural, thermodynamic, dielectric, and dynamical properties of a water system. <i>Journal of Chemical Physics</i> , 2016, 144, 114503.	1.2	23
31	Revisiting antibody modeling assessment for CDR-H3 loop. <i>Protein Engineering, Design and Selection</i> , 2016, 29, 477-484.	1.0	33
32	Flexible binding simulation by a novel and improved version of virtual-system coupled adaptive umbrella sampling. <i>Chemical Physics Letters</i> , 2016, 662, 327-332.	1.2	14
33	Variation of free-energy landscape of the p53 C-terminal domain induced by acetylation: Enhanced conformational sampling. <i>Journal of Computational Chemistry</i> , 2016, 37, 2687-2700.	1.5	25
34	The archiving and dissemination of biological structure data. <i>Current Opinion in Structural Biology</i> , 2016, 40, 17-22.	2.6	28
35	Model Building of Antibody-Antigen Complex Structures Using GBSA Scores. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 2005-2012.	2.5	16
36	Density functional study of molecular interactions in secondary structures of proteins. <i>Biophysics and Physicobiology</i> , 2016, 13, 27-35.	0.5	17

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37	Enhanced conformational sampling to visualize a free-energy landscape of protein complex formation. <i>Biochemical Journal</i> , 2016, 473, 1651-1662.	1.7	16
38	Publication of nuclear magnetic resonance experimental data with semantic web technology and the application thereof to biomedical research of proteins. <i>Journal of Biomedical Semantics</i> , 2016, 7, 16.	0.9	9
39	Elastic properties of dynein motor domain obtained from all-atom molecular dynamics simulations. <i>Protein Engineering, Design and Selection</i> , 2016, 29, 317-325.	1.0	19
40	Omokage search: shape similarity search service for biomolecular structures in both the PDB and EMDB. <i>Bioinformatics</i> , 2016, 32, 619-620.	1.8	33
41	Virtualâ€systemâ€coupled adaptive umbrella sampling to compute freeâ€energy landscape for flexible molecular docking. <i>Journal of Computational Chemistry</i> , 2015, 36, 1489-1501.	1.5	27
42	Identification of diphtheria toxin R domain mutants with enhanced inhibitory activity against HB-EGF. <i>Journal of Biochemistry</i> , 2015, 157, 331-343.	0.9	6
43	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. <i>Structure</i> , 2015, 23, 1156-1167.	1.6	159
44	Theoretical Investigation on Nearsightedness of Finite Model and Molecular Systems Based on Linear Response Function Analysis. <i>Molecules</i> , 2014, 19, 13358-13373.	1.7	7
45	The Protein Data Bank archive as an open data resource. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 1009-1014.	1.3	114
46	The zero-multipole summation method for estimating electrostatic interactions in molecular dynamics: Analysis of the accuracy and application to liquid systems. <i>Journal of Chemical Physics</i> , 2014, 140, 194307.	1.2	17
47	Structure of the Entire Stalk Region of the Dynein Motor Domain. <i>Journal of Molecular Biology</i> , 2014, 426, 3232-3245.	2.0	31
48	Highâ€resolution modeling of antibody structures by a combination of bioinformatics, expert knowledge, and molecular simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 1624-1635.	1.5	46
49	A Novel Approach of Dynamic Cross Correlation Analysis on Molecular Dynamics Simulations and Its Application to Ets1 Dimerâ€DNA Complex. <i>PLoS ONE</i> , 2014, 9, e112419.	1.1	92
50	Linear response function approach for the boundary problem of QM/MM methods. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 336-341.	1.0	8
51	How Community Has Shaped the Protein Data Bank. <i>Structure</i> , 2013, 21, 1485-1491.	1.6	33
52	The future of the protein data bank. <i>Biopolymers</i> , 2013, 99, 218-222.	1.2	65
53	Application of zero-dipole summation method to molecular dynamics simulations of a membrane protein system. <i>Chemical Physics Letters</i> , 2013, 568-569, 26-32.	1.2	50
54	Molecular Dynamics Simulations Accelerated by GPU for Biological Macromolecules with a Non-Ewald Scheme for Electrostatic Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5599-5609.	2.3	49

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55	LigandBox: A database for 3D structures of chemical compounds. <i>Biophysics (Nagoya-shi, Japan)</i> , 2013, 9, 113-121.	0.4	28
56	A virtual-system coupled multicanonical molecular dynamics simulation: Principles and applications to free-energy landscape of protein-protein interaction with an all-atom model in explicit solvent. <i>Journal of Chemical Physics</i> , 2013, 138, 184106.	1.2	32
57	Molecular Dynamics Simulations of Double-Stranded DNA in an Explicit Solvent Model with the Zero-Dipole Summation Method. <i>PLoS ONE</i> , 2013, 8, e76606.	1.1	21
58	GIRAF: a method for fast search and flexible alignment of ligand binding interfaces in proteins at atomic resolution. <i>Biophysics (Nagoya-shi, Japan)</i> , 2012, 8, 79-94.	0.4	4
59	Virtual states introduced for overcoming entropic barriers in conformational space. <i>Biophysics (Nagoya-shi, Japan)</i> , 2012, 8, 139-144.	0.4	10
60	Protein Data Bank Japan (PDBj): maintaining a structural data archive and resource description framework format. <i>Nucleic Acids Research</i> , 2012, 40, D453-D460.	6.5	126
61	Locality and nonlocality of electronic structures of molecular systems: Toward QM/MM and QM/QM approaches. <i>AIP Conference Proceedings</i> , 2012, , .	0.3	6
62	Conformational Ensembles of an Intrinsically Disordered Protein pKID with and without a KIX Domain in Explicit Solvent Investigated by All-Atom Multicanonical Molecular Dynamics. <i>Biomolecules</i> , 2012, 2, 104-121.	1.8	18
63	Computer-aided antibody design. <i>Protein Engineering, Design and Selection</i> , 2012, 25, 507-522.	1.0	203
64	Simple and accurate scheme to compute electrostatic interaction: Zero-dipole summation technique for molecular system and application to bulk water. <i>Journal of Chemical Physics</i> , 2012, 137, 054314.	1.2	45
65	Electronic and Spin Structures of the CaMn <sub>4</sub> O <sub>5</sub> (H <sub>2</sub> O) <sub>4</sub> Cluster in OEC of PSII Refined to 1.9Å... X-ray Resolution. <i>Advances in Quantum Chemistry</i> , 2012, 64, 121-187.	0.4	32
66	Non-Ewald methods: theory and applications to molecular systems. <i>Biophysical Reviews</i> , 2012, 4, 161-170.	1.5	53
67	Electron density based interaction energy estimation of the special pair in the photosynthetic reaction center. <i>Chemical Physics Letters</i> , 2012, 536, 129-135.	1.2	2
68	Enhanced and effective conformational sampling of protein molecular systems for their free energy landscapes. <i>Biophysical Reviews</i> , 2012, 4, 27-44.	1.5	60
69	Molecular dynamics scheme for precise estimation of electrostatic interaction via zero-dipole summation principle. <i>Journal of Chemical Physics</i> , 2011, 134, 164107.	1.2	83
70	A Free-Energy Landscape for Coupled Folding and Binding of an Intrinsically Disordered Protein in Explicit Solvent from Detailed All-Atom Computations. <i>Journal of the American Chemical Society</i> , 2011, 133, 10448-10458.	6.6	102
71	Selection of In Silico Drug Screening Results for G-Protein-Coupled Receptors by Using Universal Active Probes. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2398-2407.	2.5	22
72	Protein-ligand docking guided by ligand pharmacophore-mapping experiment by NMR. <i>Journal of Molecular Graphics and Modelling</i> , 2011, 31, 20-27.	1.3	12

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73	Structure determination of a protein assembly by amino acid selective cross-saturation. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 179-190.	1.5	8
74	Ab initio simulation of a 57-residue protein in explicit solvent reproduces the native conformation in the lowest free energy cluster. <i>Protein Science</i> , 2011, 20, 187-196.	3.1	17
75	Theory for trivial trajectory parallelization of multicanonical molecular dynamics and application to a polypeptide in water. <i>Journal of Computational Chemistry</i> , 2011, 32, 1286-1297.	1.5	57
76	Molecular dynamics equation designed for realizing arbitrary density: Application to sampling method utilizing the Tsallis generalized distribution. <i>Journal of Physics: Conference Series</i> , 2010, 201, 012011.	0.3	0
77	Domain distribution and intrinsic disorder in hubs in the human protein-protein interaction network. <i>Protein Science</i> , 2010, 19, 1461-1468.	3.1	62
78	PDBj Mine: design and implementation of relational database interface for Protein Data Bank Japan. <i>Database: the Journal of Biological Databases and Curation</i> , 2010, 2010, baq021-baq021.	1.4	21
79	<i>SeSAW</i> : balancing sequence and structural information in protein functional mapping. <i>Bioinformatics</i> , 2010, 26, 1258-1259.	1.8	11
80	Hub Promiscuity in Protein-Protein Interaction Networks. <i>International Journal of Molecular Sciences</i> , 2010, 11, 1930-1943.	1.8	148
81	Geometric Similarities of Protein-Protein Interfaces at Atomic Resolution Are Only Observed within Homologous Families: An Exhaustive Structural Classification Study. <i>Journal of Molecular Biology</i> , 2010, 399, 526-540.	2.0	17
82	Comprehensive Structural Classification of Ligand-Binding Motifs in Proteins. <i>Structure</i> , 2009, 17, 234-246.	1.6	43
83	Conformational requirement on peptides to exert laminin's activities and search for protein segments with laminin's activities. <i>Biopolymers</i> , 2009, 92, 124-131.	1.2	1
84	Systematic classification of CDR-L3 in antibodies: Implications of the light chain subtypes and the V <sub>L</sub> -V <sub>H</sub> interface. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 75, 139-146.	1.5	59
85	Verifying trivial parallelization of multicanonical molecular dynamics for conformational sampling of a polypeptide in explicit water. <i>Chemical Physics Letters</i> , 2009, 473, 326-329.	1.2	35
86	Intra- and Intermolecular Interaction Inducing Pyramidalization on Both Sides of a Proline Dipeptide during Isomerization: An Ab Initio QM/MM Molecular Dynamics Simulation Study in Explicit Water. <i>Journal of the American Chemical Society</i> , 2009, 131, 4535-4540.	6.6	35
87	Conformational transition states of a $\beta^2$ -hairpin peptide between the ordered and disordered conformations in explicit water. <i>Protein Science</i> , 2009, 11, 2297-2307.	3.1	72
88	Protein-inhibitor flexible docking by a multicanonical sampling: Native complex structure with the lowest free energy and a free energy barrier distinguishing the native complex from the others. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 41-53.	1.5	46
89	BioMagResBank (BMRB) as a partner in the Worldwide Protein Data Bank (wwPDB): new policies affecting biomolecular NMR depositions. <i>Journal of Biomolecular NMR</i> , 2008, 40, 153-155.	1.6	117
90	Structural classification of CDR-H3 revisited: A lesson in antibody modeling. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 73, 608-620.	1.5	113

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91	Protein structure databases with new web services for structural biology and biomedical research. <i>Briefings in Bioinformatics</i> , 2008, 9, 276-285.	3.2	81
92	Consistent Molecular Dynamics Scheme Applying the Wolf Summation for Calculating Electrostatic Interaction of Particles. <i>Journal of the Physical Society of Japan</i> , 2008, 77, 114301.	0.7	26
93	The worldwide Protein Data Bank (wwPDB): ensuring a single, uniform archive of PDB data. <i>Nucleic Acids Research</i> , 2007, 35, D301-D303.	6.5	992
94	Proteomics Research at the Institute for Protein Research, Osaka University. <i>Asia Pacific Biotech News</i> , 2007, 11, 1040-1044.	0.5	0
95	eF-seek: prediction of the functional sites of proteins by searching for similar electrostatic potential and molecular surface shape. <i>Nucleic Acids Research</i> , 2007, 35, W398-W402.	6.5	62
96	The role of charged surface residues in the binding ability of small hubs in protein-protein interaction networks. <i>Biophysics (Nagoya-shi, Japan)</i> , 2007, 3, 27-35.	0.4	10
97	Conformational sampling of a 40-residue protein consisting of $\hat{1}^{\pm}$ and $\hat{1}^2$ secondary-structure elements in explicit solvent. <i>Chemical Physics Letters</i> , 2007, 443, 364-368.	1.2	13
98	Docking of protein molecular surfaces with evolutionary trace analysis. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 69, 832-838.	1.5	23
99	ASH structure alignment package: Sensitivity and selectivity in domain classification. <i>BMC Bioinformatics</i> , 2007, 8, 116.	1.2	48
100	Similarity search for local protein structures at atomic resolution by exploiting a database management system. <i>Biophysics (Nagoya-shi, Japan)</i> , 2007, 3, 75-84.	0.4	23
101	Classification of Chemical Compounds by Protein-Compound Docking for Use in Designing a Focused Library. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 523-533.	2.9	42
102	Disordered domains and high surface charge confer hubs with the ability to interact with multiple proteins in interaction networks. <i>FEBS Letters</i> , 2006, 580, 2041-2045.	1.3	262
103	Similarities among receptor pockets and among compounds: Analysis and application to in silico ligand screening. <i>Journal of Molecular Graphics and Modelling</i> , 2005, 24, 34-45.	1.3	87
104	Deterministic design for Tsallis distribution sampling. <i>Chemical Physics Letters</i> , 2005, 405, 364-370.	1.2	2
105	Filtering high-throughput protein-protein interaction data using a combination of genomic features. <i>BMC Bioinformatics</i> , 2005, 6, 100.	1.2	138
106	GASH: an improved algorithm for maximizing the number of equivalent residues between two protein structures. <i>BMC Bioinformatics</i> , 2005, 6, 221.	1.2	26
107	Molecular dynamics sampling scheme realizing multiple distributions. <i>Physical Review E</i> , 2005, 71, 046708.	0.8	5
108	PDBML: the representation of archival macromolecular structure data in XML. <i>Bioinformatics</i> , 2005, 21, 988-992.	1.8	154



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109	Identification of the ligand binding sites on the molecular surface of proteins. <i>Protein Science</i> , 2005, 14, 711-718.	3.1	85
110	Multicanonical molecular dynamics algorithm employing an adaptive force-biased iteration scheme. <i>Physical Review E</i> , 2004, 70, 057103.	0.8	21
111	eF-site and PDBjViewer: database and viewer for protein functional sites. <i>Bioinformatics</i> , 2004, 20, 1329-1330.	1.8	113
112	Model building of a protein-protein complexed structure using saturation transfer and residual dipolar coupling without paired intermolecular NOE. <i>Journal of Biomolecular NMR</i> , 2004, 29, 325-328.	1.6	23
113	A challenge towards next-generation research infrastructure for advanced life science. <i>New Generation Computing</i> , 2004, 22, 157-166.	2.5	8
114	Modelling of third cytoplasmic loop of bovine rhodopsin by multicanonical molecular dynamics. <i>Journal of Molecular Graphics and Modelling</i> , 2004, 23, 59-68.	1.3	7
115	Structure-based prediction of DNA-binding sites on proteins Using the empirical preference of electrostatic potential and the shape of molecular surfaces. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 55, 885-894.	1.5	93
116	Detecting local structural similarity in proteins by maximizing number of equivalent residues. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 57, 381-391.	1.5	23
117	CAD $\epsilon$ -ICAD complex structure derived from saturation transfer experiment and simulated annealing without using pairwise NOE information. <i>Journal of Molecular Recognition</i> , 2004, 17, 41-50.	1.1	3
118	Free energy landscapes of small peptides in an implicit solvent model determined by force-biased multicanonical molecular dynamics simulation. <i>Chemical Physics Letters</i> , 2004, 400, 258-263.	1.2	11
119	Efficiency in the Generation of the Boltzmann $\hat{=}$ Gibbs Distribution by the Tsallis Dynamics Reweighting Method. <i>Journal of Physical Chemistry B</i> , 2004, 108, 4162-4170.	1.2	15
120	Identification of protein biochemical functions by similarity search using the molecular surface database eF-site. <i>Protein Science</i> , 2003, 12, 1589-1595.	3.1	156
121	Protein informatics towards function identification. <i>Current Opinion in Structural Biology</i> , 2003, 13, 396-400.	2.6	64
122	$\beta$ -Hairpins, $\beta$ -helices, and the intermediates among the secondary structures in the energy landscape of a peptide from a distal $\beta$ -hairpin of SH3 domain. <i>Journal of Computational Chemistry</i> , 2003, 24, 310-318.	1.5	30
123	Deterministic generation of the Boltzmann $\hat{=}$ Gibbs distribution and the free energy calculation from the Tsallis distribution. <i>Chemical Physics Letters</i> , 2003, 382, 367-373.	1.2	9
124	Announcing the worldwide Protein Data Bank. <i>Nature Structural and Molecular Biology</i> , 2003, 10, 980-980.	3.6	2,355
125	The Filling Potential Method: A Method for Estimating the Free Energy Surface for Protein $\hat{=}$ Ligand Docking. <i>Journal of Physical Chemistry B</i> , 2003, 107, 13201-13210.	1.2	139
126	Crystal structure of the conserved protein TT1542 from <i>Thermus thermophilus</i> HB8. <i>Protein Science</i> , 2003, 12, 1621-1632.	3.1	32



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127	Determination of multicanonical weight based on a stochastic model of sampling dynamics. <i>Physical Review E</i> , 2003, 68, 021110.	0.8	23
128	Tsallis dynamics using the Nosé-Hoover approach. <i>Physical Review E</i> , 2002, 65, 026105.	0.8	33
129	Calibration of force-field dependency in free energy landscapes of peptide conformations by quantum chemical calculations. <i>Journal of Computational Chemistry</i> , 2002, 23, 470-476.	1.5	13
130	A method of comparing protein molecular surface based on normal vectors with attributes and its application to function identification. <i>Information Sciences</i> , 2002, 146, 41-54.	4.0	6
131	A filtering method for high-speed retrieval of similar active sites. <i>Information Sciences</i> , 2002, 146, 55-65.	4.0	0
132	Identification of protein functions from a molecular surface database, eF-site. <i>Journal of Structural and Functional Genomics</i> , 2002, 2, 9-22.	1.2	111
133	Energy landscape of a $\beta$ -hairpin peptide in explicit water studied by multicanonical molecular dynamics. <i>Chemical Physics Letters</i> , 2001, 337, 169-175.	1.2	38
134	Energy landscape of a peptide consisting of $\alpha$ -helix, $\beta$ -helix, $\beta$ -turn, $\beta$ -hairpin, and other disordered conformations. <i>Protein Science</i> , 2001, 10, 1160-1171.	3.1	80
135	A Role of the Third Complementarity-determining Region in the Affinity Maturation of an Antibody. <i>Journal of Biological Chemistry</i> , 2001, 276, 27622-27628.	1.6	39
136	Peptide free-energy profile is strongly dependent on the force field: Comparison of C96 and AMBER95. <i>Journal of Computational Chemistry</i> , 2000, 21, 748-762.	1.5	60
137	Free energy landscapes of peptides by enhanced conformational sampling 1 Edited by B. Honig. <i>Journal of Molecular Biology</i> , 2000, 296, 197-216.	2.0	58
138	The multicanonical weighted histogram analysis method for the free-energy landscape along structural transition paths. <i>Chemical Physics Letters</i> , 1999, 312, 247-254.	1.2	36
139	Enhanced conformational diversity search of CDR-H3 in antibodies: Role of the first CDR-H3 residue. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 37, 683-696.	1.5	36
140	H3-rules: identification of CDR-H3 structures in antibodies. <i>FEBS Letters</i> , 1999, 455, 188-197.	1.3	151
141	A general <i>ab initio</i> approach for free energy landscapes of biological molecules around the transition states. <i>Proceedings of the Japan Academy Series B: Physical and Biological Sciences</i> , 1999, 75, 291-294.	1.6	3
142	Thermodynamics of specific and non-specific DNA binding by the c-myb DNA-binding domain. <i>Journal of Molecular Biology</i> , 1998, 276, 571-590.	2.0	100
143	Conformational sampling of CDR-H3 in antibodies by multicanonical molecular dynamics simulation 1 Edited by I. A. Wilson. <i>Journal of Molecular Biology</i> , 1998, 278, 481-496.	2.0	58
144	Multicanonical Ensemble Generated by Molecular Dynamics Simulation for Enhanced Conformational Sampling of Peptides. <i>Journal of Physical Chemistry B</i> , 1997, 101, 817-824.	1.2	388

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145	Two-component multicanonical Monte Carlo method for effective conformation sampling. <i>Journal of Computational Chemistry</i> , 1997, 18, 2086-2092.	1.5	67
146	Ab initio MO study of the chlorophyll dimer in the photosynthetic reaction center. I. A theoretical treatment of the electrostatic field created by the surrounding proteins. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 137-151.	1.0	36
147	Flexible docking of a ligand peptide to a receptor protein by multicanonical molecular dynamics simulation. <i>Chemical Physics Letters</i> , 1997, 278, 297-301.	1.2	85
148	Structural classification of CDR-H3 in antibodies. <i>FEBS Letters</i> , 1996, 399, 1-8.	1.3	207
149	Roles of electrostatic interaction in proteins. <i>Quarterly Reviews of Biophysics</i> , 1996, 29, 1-90.	2.4	278
150	Presto(protein engineering simulator): A vectorized molecular mechanics program for biopolymers. <i>Computers &amp; Chemistry</i> , 1992, 16, 243-248.	1.2	179
151	Numerical Calculations of Electrostatic Potentials of Protein-Solvent Systems by the Self Consistent Boundary Method. <i>Journal of the Physical Society of Japan</i> , 1987, 56, 1609-1622.	0.7	77
152	Nature of the Charge Distribution in Proteins. III. Electric Multipole Structures. <i>Journal of the Physical Society of Japan</i> , 1985, 54, 4047-4052.	0.7	18
153	Nature of the Charge Distribution in Proteins. II. Effect of Atomic Partial Charges on Ionic Charges. <i>Journal of the Physical Society of Japan</i> , 1985, 54, 4042-4046.	0.7	10
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