# Haruki Nakamura

List of Publications by Year
in descending order



| 157 | 12,394 | 36271 51 | 27389 106 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 164 | 164 | 164 | 12326 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Difference of binding modes among three ligands to a receptor mSin3B corresponding to their inhibitory activities. Scientific Reports, 2021, 11, 6178. | 1.6 | 10 |
| 2 | Announcing changes to the publishing procedures of â€œBiophysics and Physicobiologyâ€•(BPPB)â€”the Biophysical Society of Japanâ€™s English language biophysics journal. Biophysical Reviews, 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. Journal of Chemical Information and Modeling, 2020, 60, 4867-4880. | 2.5 | 13 |
| 4 | Big data science at AMED-BINDS. Biophysical Reviews, 2020, 12, 221-224. | 1.5 | 5 |
| 5 | Editorial for the Special Issue of Biophysical Reviews focused on the Biophysical Society of Japan with select scientific content from the 57th BSJ annual meeting, Miyazaki, Japan. Biophysical Reviews, 2020, 12, 183-185. | 1.5 | 11 |
| 6 | How A Novel Scientific Concept Was Coined the â€œMolten Globule Stateâ€• Biomolecules, 2020, 10, 269. | 1.8 | 13 |
| 7 | myPresto/omegagene 2020: a molecular dynamics simulation engine for virtual-system coupled sampling. Biophysics and Physicobiology, 2020, 17, 140-146. | 0.5 | 8 |
| 8 | The Papers that Influenced My Career: Creamer and Rose. Seibutsu Butsuri, 2020, 60, 190-191. | 0.0 | 0 |
| 9 | Multidimensional virtualâ€•system coupled canonical molecular dynamics to compute freeâ€•energy landscapes of peptide multimer assembly. Journal of Computational Chemistry, 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. Protein Engineering, Design and Selection, 2019, 32, 297-308. | 1.0 | 15 |
| 11 | Hydrogen bond donors and acceptors are generally depolarized in Î±â€•helices as revealed by a molecular tailoring approach. Journal of Computational Chemistry, 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. Journal of Chemical Theory and Computation, 2019, 15, 2597-2607. | 2.3 | 14 |
| 13 | Protein Data Bank: the single global archive for 3D macromolecular structure data. Nucleic Acids Research, 2019, 47, D520-D528. | 6.5 | 671 |
| 14 | Molecular dynamics coupled with a virtual system for effective conformational sampling. Journal of Computational Chemistry, 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. Nucleic Acids Research, 2018, 46, 2243-2251. | 6.5 | 34 |
| 16 | Foreword to â€˜Multiscale structural biology: biophysical principles and mechanisms underlying the action of bio-nanomachinesâ€™, a special issue in Honour of Fumio Arisakaâ€™s 70th birthday. Biophysical Reviews, 2018, 10, 105-129. | 1.5 | 4 |
| 17 | Data Science and PDBj Activities. Seibutsu Butsuri, 2018, 58, 071-077. | 0.0 | 0 |
| 18 | New tools and functions in dataâ€•out activities at Protein Data Bank Japan (PDBj). Protein Science, 2018, 27, 95-102. | 3.1 | 90 |

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| 19 | Overall Introduction and Rationale, with View from Computational Biology. Advances in Experimental Medicine and Biology, 2018, 1105, 3-9. | 0.8 | 1 |
| 20 | Worldwide Protein Data Bank biocuration supporting open access to high-quality 3D structural biology data. Database: the Journal of Biological Databases and Curation, 2018, 2018, . | 1.4 | 45 |
| 21 | OneDep: Unified wwPDB System for Deposition, Biocuration, and Validation of Macromolecular Structures in the PDB Archive. Structure, 2017, 25, 536-545. | 1.6 | 130 |
| 22 | Accurate Prediction of Complex Structure and Affinity for a Flexible Protein Receptor and Its Inhibitor. Journal of Chemical Theory and Computation, 2017, 13, 2389-2399. | 2.3 | 43 |
| 23 | Protein Data Bank (PDB): The Single Global Macromolecular Structure Archive. Methods in Molecular Biology, 2017, 1607, 627-641. | 0.4 | 592 |
| 24 | PDB-Dev: a Prototype System for Depositing Integrative/Hybrid Structural Models. Structure, 2017, 25, 1317-1318. | 1.6 | 84 |
| 25 | Validation of Structures in the Protein Data Bank. Structure, 2017, 25, 1916-1927. | 1.6 | 210 |
| 26 | Protein Data Bank Japan (PDBj): updated user interfaces, resource description framework, analysis tools for large structures. Nucleic Acids Research, 2017, 45, D282-D288. | 6.5 | 108 |
| 27 | Enhancement of canonical sampling by virtual-state transitions. Journal of Chemical Physics, 2017, 146, 044104. | 1.2 | 12 |
| 28 | Multi-dimensional virtual system introduced to enhance canonical sampling. Journal of Chemical Physics, 2017, 147, 134102. | 1.2 | 8 |
| 29 | Molmil: a molecular viewer for the PDB and beyond. Journal of Cheminformatics, 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. Journal of Chemical Physics, 2016, 144, 114503. | 1.2 | 23 |
| 31 | Revisiting antibody modeling assessment for CDR-H3 loop. Protein Engineering, Design and Selection, 2016, 29, 477-484. | 1.0 | 33 |
| 32 | Flexible binding simulation by a novel and improved version of virtual-system coupled adaptive umbrella sampling. Chemical Physics Letters, 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. Journal of Computational Chemistry, 2016, 37, 2687-2700. | 1.5 | 25 |
| 34 | The archiving and dissemination of biological structure data. Current Opinion in Structural Biology, 2016, 40, 17-22. | 2.6 | 28 |
| 35 | Model Building of Antibodyâ€“Antigen Complex Structures Using GBSA Scores. Journal of Chemical Information and Modeling, 2016, 56, 2005-2012. | 2.5 | 16 |
| 36 | Density functional study of molecular interactions in secondary structures of proteins. Biophysics and Physicobiology, 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. Biochemical Journal, 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. Journal of Biomedical Semantics, 2016, 7, 16. | 0.9 | 9 |
| 39 | Elastic properties of dynein motor domain obtained from all-atom molecular dynamics simulations. Protein Engineering, Design and Selection, 2016, 29, 317-325. | 1.0 | 19 |
| 40 | Omokage search: shape similarity search service for biomolecular structures in both the PDB and EMDB. Bioinformatics, 2016, 32, 619-620. | 1.8 | 33 |
| 41 | Virtualâ€systemâ€coupled adaptive umbrella sampling to compute freeâ€energy landscape for flexible molecular docking. Journal of Computational Chemistry, 2015, 36, 1489-1501. | 1.5 | 27 |
| 42 | Identification of diphtheria toxin R domain mutants with enhanced inhibitory activity against HB-EGF. Journal of Biochemistry, 2015, 157, 331-343. | 0.9 | 6 |
| 43 | Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. Structure, 2015, 23, 1156-1167. | 1.6 | 159 |
| 44 | Theoretical Investigation on Nearsightedness of Finite Model and Molecular Systems Based on Linear Response Function Analysis. Molecules, 2014, 19, 13358-13373. | 1.7 | 7 |
| 45 | The Protein Data Bank archive as an open data resource. Journal of Computer-Aided Molecular Design, 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. Journal of Chemical Physics, 2014, 140, 194307. | 1.2 | 17 |
| 47 | Structure of the Entire Stalk Region of the Dynein Motor Domain. Journal of Molecular Biology, 2014, 426, 3232-3245. | 2.0 | 31 |
| 48 | Highâ€resolution modeling of antibody structures by a combination of bioinformatics, expert knowledge, and molecular simulations. Proteins: Structure, Function and Bioinformatics, 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. PLoS ONE, 2014, 9, e112419. | 1.1 | 92 |
| 50 | Linear response function approach for the boundary problem of QM/MM methods. International Journal of Quantum Chemistry, 2013, 113, 336-341. | 1.0 | 8 |
| 51 | How Community Has Shaped the Protein Data Bank. Structure, 2013, 21, 1485-1491. | 1.6 | 33 |
| 52 | The future of the protein data bank. Biopolymers, 2013, 99, 218-222. | 1.2 | 65 |
| 53 | Application of zero-dipole summation method to molecular dynamics simulations of a membrane protein system. Chemical Physics Letters, 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. Journal of Chemical Theory and Computation, 2013, 9, 5599-5609. | 2.3 | 49 |

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| 55 | LigandBox: A database for 3D structures of chemical compounds. Biophysics (Nagoya-shi, Japan), 2013, 9, 113-121. | 0.4 | 28 |
| 56 | A virtual-system coupled multicanonical molecular dynamics simulation: Principles and applications to free-energy landscape of proteinâ€“protein interaction with an all-atom model in explicit solvent. Journal of Chemical Physics, 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. PLoS ONE, 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. Biophysics (Nagoya-shi, Japan), 2012, 8, 79-94. | 0.4 | 4 |
| 59 | Virtual states introduced for overcoming entropic barriers in conformational space. Biophysics (Nagoya-shi, Japan), 2012, 8, 139-144. | 0.4 | 10 |
| 60 | Protein Data Bank Japan (PDBj): maintaining a structural data archive and resource description framework format. Nucleic Acids Research, 2012, 40, D453-D460. | 6.5 | 126 |
| 61 | Locality and nonlocality of electronic structures of molecular systems: Toward QM/MM and QM/QM approaches. AIP Conference Proceedings, 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. Biomolecules, 2012, 2, 104-121. | 1.8 | 18 |
| 63 | Computer-aided antibody design. Protein Engineering, Design and Selection, 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. Journal of Chemical Physics, 2012, 137, 054314. | 1.2 | 45 |
| 65 | Electronic and Spin Structures of the CaMn4O5(H2O)4 Cluster in OEC of PSII Refined to 1.9Ã... X-ray Resolution. Advances in Quantum Chemistry, 2012, 64, 121-187. | 0.4 | 32 |
| 66 | Non-Ewald methods: theory and applications to molecular systems. Biophysical Reviews, 2012, 4, 161-170. | 1.5 | 53 |
| 67 | Electron density based interaction energy estimation of the special pair in the photosynthetic reaction center. Chemical Physics Letters, 2012, 536, 129-135. | 1.2 | 2 |
| 68 | Enhanced and effective conformational sampling of protein molecular systems for their free energy landscapes. Biophysical Reviews, 2012, 4, 27-44. | 1.5 | 60 |
| 69 | Molecular dynamics scheme for precise estimation of electrostatic interaction via zero-dipole summation principle. Journal of Chemical Physics, 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. Journal of the American Chemical Society, 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. Journal of Chemical Information and Modeling, 2011, 51, 2398-2407. | 2.5 | 22 |
| 72 | Proteinâ€“ligand docking guided by ligand pharmacophore-mapping experiment by NMR. Journal of Molecular Graphics and Modelling, 2011, 31, 20-27. | 1.3 | 12 |

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| 73 | Structure determination of a protein assembly by amino acid selective crossâ€saturation. Proteins: Structure, Function and Bioinformatics, 2011, 79, 179-190. | 1.5 | 8 |
| 74 | Ab initio simulation of a 57â€residue protein in explicit solvent reproduces the native conformation in the lowest freeâ€energy cluster. Protein Science, 2011, 20, 187-196. | 3.1 | 17 |
| 75 | Theory for trivial trajectory parallelization of multicanonical molecular dynamics and application to a polypeptide in water. Journal of Computational Chemistry, 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. Journal of Physics: Conference Series, 2010, 201, 012011. | 0.3 | 0 |
| 77 | Domain distribution and intrinsic disorder in hubs in the human proteinâ€“protein interaction network. Protein Science, 2010, 19, 1461-1468. | 3.1 | 62 |
| 78 | PDBj Mine: design and implementation of relational database interface for Protein Data Bank Japan. Database: the Journal of Biological Databases and Curation, 2010, 2010, baq021-baq021. | 1.4 | 21 |
| 79 | SeSAW: balancing sequence and structural information in protein functional mapping. Bioinformatics, 2010, 26, 1258-1259. | 1.8 | 11 |
| 80 | Hub Promiscuity in Protein-Protein Interaction Networks. International Journal of Molecular Sciences, 2010, 11, 1930-1943. | 1.8 | 148 |
| 81 | Geometric Similarities of Proteinâ€“Protein Interfaces at Atomic Resolution Are Only Observed within Homologous Families: An Exhaustive Structural Classification Study. Journal of Molecular Biology, 2010, 399, 526-540. | 2.0 | 17 |
| 82 | Comprehensive Structural Classification of Ligand-Binding Motifs in Proteins. Structure, 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. Biopolymers, 2009, 92, 124-131. | 1.2 | 1 |
| 84 | Systematic classification of CDRâ€L3 in antibodies: Implications of the light chain subtypes and the V<sub>L</sub>â€“V<sub>H</sub> interface. Proteins: Structure, Function and Bioinformatics, 2009, 75, 139-146. | 1.5 | 59 |
| 85 | Verifying trivial parallelization of multicanonical molecular dynamics for conformational sampling of a polypeptide in explicit water. Chemical Physics Letters, 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. Journal of the American Chemical Society, 2009, 131, 4535-4540. | 6.6 | 35 |
| 87 | Conformational transition states of a Î²-hairpin peptide between the ordered and disordered conformations in explicit water. Protein Science, 2009, 11, 2297-2307. | 3.1 | 72 |
| 88 | Proteinâ€inhibitor flexible docking by a multicanonical sampling: Native complex structure with the lowest free energy and a freeâ€energy barrier distinguishing the native complex from the others. Proteins: Structure, Function and Bioinformatics, 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. Journal of Biomolecular NMR, 2008, 40, 153-155. | 1.6 | 117 |
| 90 | Structural classification of CDRâ€H3 revisited: A lesson in antibody modeling. Proteins: Structure, Function and Bioinformatics, 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. Briefings in Bioinformatics, 2008, 9, 276-285. | 3.2 | 81 |
| 92 | Consistent Molecular Dynamics Scheme Applying the Wolf Summation for Calculating Electrostatic Interaction of Particles. Journal of the Physical Society of Japan, 2008, 77, 114301. | 0.7 | 26 |
| 93 | The worldwide Protein Data Bank (wwPDB): ensuring a single, uniform archive of PDB data. Nucleic Acids Research, 2007, 35, D301-D303. | 6.5 | 992 |
| 94 | Proteomics Research at the Institute for Protein Research, Osaka University. Asia Pacific Biotech News, 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. Nucleic Acids Research, 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. Biophysics (Nagoya-shi, Japan), 2007, 3, 27-35. | 0.4 | 10 |
| 97 | Conformational sampling of a 40-residue protein consisting of Î± and Î² secondary-structure elements in explicit solvent. Chemical Physics Letters, 2007, 443, 364-368. | 1.2 | 13 |
| 98 | Docking of protein molecular surfaces with evolutionary trace analysis. Proteins: Structure, Function and Bioinformatics, 2007, 69, 832-838. | 1.5 | 23 |
| 99 | ASH structure alignment package: Sensitivity and selectivity in domain classification. BMC Bioinformatics, 2007, 8, 116. | 1.2 | 48 |
| 100 | Similarity search for local protein structures at atomic resolution by exploiting a database management system. Biophysics (Nagoya-shi, Japan), 2007, 3, 75-84. | 0.4 | 23 |
| 101 | Classification of Chemical Compounds by Proteinâ^'Compound Docking for Use in Designing a Focused Library. Journal of Medicinal Chemistry, 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. FEBS Letters, 2006, 580, 2041-2045. | 1.3 | 262 |
| 103 | Similarities among receptor pockets and among compounds: Analysis and application to in silico ligand screening. Journal of Molecular Graphics and Modelling, 2005, 24, 34-45. | 1.3 | 87 |
| 104 | Deterministic design for Tsallis distribution sampling. Chemical Physics Letters, 2005, 405, 364-370. | 1.2 | 2 |
| 105 | Filtering high-throughput protein-protein interaction data using a combination of genomic features. BMC Bioinformatics, 2005, 6, 100. | 1.2 | 138 |
| 106 | GASH: an improved algorithm for maximizing the number of equivalent residues between two protein structures. BMC Bioinformatics, 2005, 6, 221. | 1.2 | 26 |
| 107 | Molecular dynamics sampling scheme realizing multiple distributions. Physical Review E, 2005, 71, 046708. | 0.8 | 5 |
| 108 | PDBML: the representation of archival macromolecular structure data in XML. Bioinformatics, 2005, 21, 988-992. | 1.8 | 154 |

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| 109 | Identification of the ligand binding sites on the molecular surface of proteins. Protein Science, 2005, 14, 711-718. | 3.1 | 85 |
| 110 | Multicanonical molecular dynamics algorithm employing an adaptive force-biased iteration scheme. Physical Review E, 2004, 70, 057103. | 0.8 | 21 |
| 111 | eF-site and PDBjViewer: database and viewer for protein functional sites. Bioinformatics, 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. Journal of Biomolecular NMR, 2004, 29, 325-328. | 1.6 | 23 |
| 113 | A challenge towards next-generation research infrastructure for advanced life science. New Generation Computing, 2004, 22, 157-166. | 2.5 | 8 |
| 114 | Modelling of third cytoplasmic loop of bovine rhodopsin by multicanonical molecular dynamics. Journal of Molecular Graphics and Modelling, 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. Proteins: Structure, Function and Bioinformatics, 2004, 55, 885-894. | 1.5 | 93 |
| 116 | Detecting local structural similarity in proteins by maximizing number of equivalent residues. Proteins: Structure, Function and Bioinformatics, 2004, 57, 381-391. | 1.5 | 23 |
| 117 | CADâ€“ICAD complex structure derived from saturation transfer experiment and simulated annealing without using pairwise NOE information. Journal of Molecular Recognition, 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. Chemical Physics Letters, 2004, 400, 258-263. | 1.2 | 11 |
| 119 | Efficiency in the Generation of the Boltzmannâ^'Gibbs Distribution by the Tsallis Dynamics Reweighting Method. Journal of Physical Chemistry B, 2004, 108, 4162-4170. | 1.2 | 15 |
| 120 | Identification of protein biochemical functions by similarity search using the molecular surface database eF-site. Protein Science, 2003, 12, 1589-1595. | 3.1 | 156 |
| 121 | Protein informatics towards function identification. Current Opinion in Structural Biology, 2003, 13, 396-400. | 2.6 | 64 |
| 122 | ?-Hairpins, ?-helices, and the intermediates among the secondary structures in the energy landscape of a peptide from a distal ?-hairpin of SH3 domain. Journal of Computational Chemistry, 2003, 24, 310-318. | 1.5 | 30 |
| 123 | Deterministic generation of the Boltzmannâ€“Gibbs distribution and the free energy calculation from the Tsallis distribution. Chemical Physics Letters, 2003, 382, 367-373. | 1.2 | 9 |
| 124 | Announcing the worldwide Protein Data Bank. Nature Structural and Molecular Biology, 2003, 10, 980-980. | 3.6 | 2,355 |
| 125 | The Filling Potential Method:Â A Method for Estimating the Free Energy Surface for Proteinâ^'Ligand Docking. Journal of Physical Chemistry B, 2003, 107, 13201-13210. | 1.2 | 139 |
| 126 | Crystal structure of the conserved protein TT1542 from Thermus thermophilus HB8. Protein Science, 2003, 12, 1621-1632. | 3.1 | 32 |

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| 127 | Determination of multicanonical weight based on a stochastic model of sampling dynamics. Physical Review E, 2003, 68, 021110. | 0.8 | 23 |
| 128 | Tsallis dynamics using the NosÃ©-Hoover approach. Physical Review E, 2002, 65, 026105. | 0.8 | 33 |
| 129 | Calibration of force-field dependency in free energy landscapes of peptide conformations by quantum chemical calculations. Journal of Computational Chemistry, 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. Information Sciences, 2002, 146, 41-54. | 4.0 | 6 |
| 131 | A filtering method for high-speed retrieval of similar active sites. Information Sciences, 2002, 146, 55-65. | 4.0 | 0 |
| 132 | Identification of protein functions from a molecular surface database, eF-site. Journal of Structural and Functional Genomics, 2002, 2, 9-22. | 1.2 | 111 |
| 133 | Energy landscape of a Î²-hairpin peptide in explicit water studied by multicanonical molecular dynamics. Chemical Physics Letters, 2001, 337, 169-175. | 1.2 | 38 |
| 134 | Energy landscape of a peptide consisting of Î±-helix, 310-helix, Î²-turn, Î²-hairpin, and other disordered conformations. Protein Science, 2001, 10, 1160-1171. | 3.1 | 80 |
| 135 | A Role of the Third Complementarity-determining Region in the Affinity Maturation of an Antibody. Journal of Biological Chemistry, 2001, 276, 27622-27628. | 1.6 | 39 |
| 136 | Peptide free-energy profile is strongly dependent on the force field: Comparison of C96 and AMBER95. Journal of Computational Chemistry, 2000, 21, 748-762. | 1.5 | 60 |
| 137 | Free energy landscapes of peptides by enhanced conformational sampling 1 1Edited by B. Honig. Journal of Molecular Biology, 2000, 296, 197-216. | 2.0 | 58 |
| 138 | The multicanonical weighted histogram analysis method for the free-energy landscape along structural transition paths. Chemical Physics Letters, 1999, 312, 247-254. | 1.2 | 36 |
| 139 | Enhanced conformational diversity search of CDR-H3 in antibodies: Role of the first CDR-H3 residue. Proteins: Structure, Function and Bioinformatics, 1999, 37, 683-696. | 1.5 | 36 |
| 140 | H3-rules: identification of CDR-H3 structures in antibodies. FEBS Letters, 1999, 455, 188-197. | 1.3 | 151 |
| 141 | A general ab initio approach for free energy landscapes of biological molecules around the transition states. Proceedings of the Japan Academy Series B: Physical and Biological Sciences, 1999, 75, 291-294. | 1.6 | 3 |
| 142 | Thermodynamics of specific and non-specific DNA binding by the c-myb DNA-binding domain. Journal of Molecular Biology, 1998, 276, 571-590. | 2.0 | 100 |
| 143 | Conformational sampling of CDR-H3 in antibodies by multicanonical molecular dynamics simulation 1 1Edited by I. A. Wilson. Journal of Molecular Biology, 1998, 278, 481-496. | 2.0 | 58 |
| 144 | Multicanonical Ensemble Generated by Molecular Dynamics Simulation for Enhanced Conformational Sampling of Peptides. Journal of Physical Chemistry B, 1997, 101, 817-824. | 1.2 | 388 |

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| 145 | Two-component multicanonical Monte Carlo method for effective conformation sampling. Journal of Computational Chemistry, 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. International Journal of Quantum Chemistry, 1997, 61, 137-151. | 1.0 | 36 |
| 147 | Flexible docking of a ligand peptide to a receptor protein by multicanonical molecular dynamics simulation. Chemical Physics Letters, 1997, 278, 297-301. | 1.2 | 85 |
| 148 | Structural classification of CDR-H3 in antibodies. FEBS Letters, 1996, 399, 1-8. | 1.3 | 207 |
| 149 | Roles of electrostatic interaction in proteins. Quarterly Reviews of Biophysics, 1996, 29, 1-90. | 2.4 | 278 |
| 150 | Presto(protein engineering simulator): A vectorized molecular mechanics program for biopolymers. Computers & Chemistry, 1992, 16, 243-248. | 1.2 | 179 |
| 151 | Numerical Calculations of Electrostatic Potentials of Protein-Solvent Systems by the Self Consistent Boundary Method. Journal of the Physical Society of Japan, 1987, 56, 1609-1622. | 0.7 | 77 |
| 152 | Nature of the Charge Distribution in Proteins. III. Electric Multipole Structures. Journal of the Physical Society of Japan, 1985, 54, 4047-4052. | 0.7 | 18 |
| 153 | Nature of the Charge Destribution in Proteins. II. Effect of Atomic Partial Charges on Ionic Charges. Journal of the Physical Society of Japan, 1985, 54, 4042-4046. | 0.7 | 10 |
| 154 | Electrostatic Complementarities between Guest Ligands and Host Enzymes. Journal of the Physical Society of Japan, 1985, 54, 3257-3260. | 0.7 | 10 |
| 155 | Applications of molecular graphics to biophysics.. Seibutsu Butsuri, 1985, 25, 1-10. | 0.0 | 1 |
| 156 | Nature of the charge distribution in proteins. Nature, 1981, 293, 757-758. | 13.7 | 140 |
| 157 | Nearsightedness-related indices of finite systems based on linear response function: one-dimensional cases. Molecular Physics, 0, , 1-9. | 0.8 | 2 |