Shoji Takada

List of Publications by Year in descending order

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140 6,315 37
papers citations h-index

162 162 162 4717 all docs docs citations times ranked citing authors

75

g-index

| # | Article | IF | CITATIONS |
|----|---|------|-----------|
| 1 | On the Hamiltonian replica exchange method for efficient sampling of biomolecular systems: Application to protein structure prediction. Journal of Chemical Physics, 2002, 116, 9058-9067. | 3.0 | 681 |
| 2 | Roles of native topology and chain-length scaling in protein folding: A simulation study with a GÅ-like model 1 1Edited by B. Honig. Journal of Molecular Biology, 2001, 313, 171-180. | 4.2 | 344 |
| 3 | Dynamic energy landscape view of coupled binding and protein conformational change: Induced-fit versus population-shift mechanisms. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 11182-11187. | 7.1 | 297 |
| 4 | Multiple-basin energy landscapes for large-amplitude conformational motions of proteins: Structure-based molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 11844-11849. | 7.1 | 286 |
| 5 | Bimodal protein solubility distribution revealed by an aggregation analysis of the entire ensemble of <i>Escherichia coli</i> proteins. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 4201-4206. | 7.1 | 253 |
| 6 | Coarse-grained molecular simulations of large biomolecules. Current Opinion in Structural Biology, 2012, 22, 130-137. | 5.7 | 205 |
| 7 | How protein thermodynamics and folding mechanisms are altered by the chaperonin cage: Molecular simulations. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 11367-11372. | 7.1 | 204 |
| 8 | CafeMol: A Coarse-Grained Biomolecular Simulator for Simulating Proteins at Work. Journal of Chemical Theory and Computation, 2011, 7, 1979-1989. | 5.3 | 202 |
| 9 | Folding dynamics with nonadditive forces: A simulation study of a designed helical protein and a random heteropolymer. Journal of Chemical Physics, 1999, 110, 11616-11629. | 3.0 | 188 |
| 10 | Microscopic theory of protein folding rates. II. Local reaction coordinates and chain dynamics. Journal of Chemical Physics, 2001, 114, 5082-5096. | 3.0 | 164 |
| 11 | Energy landscape views for interplays among folding, binding, and allostery of calmodulin domains. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 10550-10555. | 7.1 | 150 |
| 12 | Frustration, specific sequence dependence, and nonlinearity in large-amplitude fluctuations of allosteric proteins. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3504-3509. | 7.1 | 143 |
| 13 | Energy landscape and multiroute folding of topologically complex proteins adenylate kinase and 2ouf-knot. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 17789-17794. | 7.1 | 134 |
| 14 | Modeling Structural Dynamics of Biomolecular Complexes by Coarse-Grained Molecular Simulations. Accounts of Chemical Research, 2015, 48, 3026-3035. | 15.6 | 134 |
| 15 | On easy implementation of a variant of the replica exchange with solute tempering in GROMACS. Journal of Computational Chemistry, 2011, 32, 1228-1234. | 3.3 | 131 |
| 16 | Folding-based molecular simulations reveal mechanisms of the rotary motor F1-ATPase. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 5367-5372. | 7.1 | 116 |
| 17 | Effects of vibrational excitation on multidimensional tunneling: General study and proton tunneling in tropolone. Journal of Chemical Physics, 1995, 102, 3977-3992. | 3.0 | 103 |
| 18 | Microscopic theory of protein folding rates. I. Fine structure of the free energy profile and folding routes from a variational approach. Journal of Chemical Physics, 2001, 114, 5069-5081. | 3.0 | 99 |

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| 19 | Multiscale Ensemble Modeling of Intrinsically Disordered Proteins: p53 N-Terminal Domain. Biophysical Journal, 2011, 101, 1450-1458. | 0.5 | 92 |
| 20 | p53 Searches on DNA by Rotation-Uncoupled Sliding at C-Terminal Tails and Restricted Hopping of Core Domains. Journal of the American Chemical Society, 2012, 134, 14555-14562. | 13.7 | 89 |
| 21 | Optimizing physical energy functions for protein folding. Proteins: Structure, Function and Bioinformatics, 2003, 54, 88-103. | 2.6 | 84 |
| 22 | Wentzel–Kramers–Brillouin theory of multidimensional tunneling: General theory for energy splitting. Journal of Chemical Physics, 1994, 100, 98-113. | 3.0 | 83 |
| 23 | Drug export and allosteric coupling in a multidrug transporter revealed by molecular simulations. Nature Communications, 2010, $1,117.$ | 12.8 | 82 |
| 24 | De Novo Design of Foldable Proteins with Smooth Folding Funnel. Structure, 2003, 11, 581-590. | 3.3 | 77 |
| 25 | DNA sliding in nucleosomes via twist defect propagation revealed by molecular simulations. Nucleic Acids Research, 2018, 46, 2788-2801. | 14.5 | 77 |
| 26 | Partial Unwrapping and Histone Tail Dynamics in Nucleosome Revealed by Coarse-Grained Molecular Simulations. PLoS Computational Biology, 2015, 11, e1004443. | 3.2 | 73 |
| 27 | Folding energy landscape and network dynamics of small globular proteins. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 73-78. | 7.1 | 68 |
| 28 | Dynamic Coupling among Protein Binding, Sliding, and DNA Bending Revealed by Molecular Dynamics. Journal of the American Chemical Society, 2016, 138, 8512-8522. | 13.7 | 63 |
| 29 | Nucleosome allostery in pioneer transcription factor binding. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 20586-20596. | 7.1 | 57 |
| 30 | Adenosine Triphosphate Hydrolysis Mechanism in Kinesin Studied by Combined Quantum-Mechanical/Molecular-Mechanical Metadynamics Simulations. Journal of the American Chemical Society, 2013, 135, 8908-8919. | 13.7 | 56 |
| 31 | Near-atomic structural model for bacterial DNA replication initiation complex and its functional insights. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E8021-E8030. | 7.1 | 56 |
| 32 | Drug Uptake Pathways of Multidrug Transporter AcrB Studied by Molecular Simulations and Site-Directed Mutagenesis Experiments. Journal of the American Chemical Society, 2013, 135, 7474-7485. | 13.7 | 53 |
| 33 | Guiding the search for a protein's maximum rate of folding. Chemical Physics, 2004, 307, 99-109. | 1.9 | 52 |
| 34 | Sequence-dependent nucleosome sliding in rotation-coupled and uncoupled modes revealed by molecular simulations. PLoS Computational Biology, 2017, 13, e1005880. | 3.2 | 50 |
| 35 | Protein folding simulation with solvent-induced force field: Folding pathway ensemble of three-helix-bundle proteins. Proteins: Structure, Function and Bioinformatics, 2001, 42, 85-98. | 2.6 | 47 |
| 36 | A reversible fragment assembly method for de novo protein structure prediction. Journal of Chemical Physics, 2003, 119, 6895-6903. | 3.0 | 46 |

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| 37 | SimFold energy function for de novo protein structure prediction: Consensus with Rosetta. Proteins: Structure, Function and Bioinformatics, 2005, 62, 381-398. | 2.6 | 46 |
| 38 | Gŕmodel revisited. Biophysics and Physicobiology, 2019, 16, 248-255. | 1.0 | 40 |
| 39 | Coarse-Grained Structure-Based Model for RNA-Protein Complexes Developed by Fluctuation Matching. Journal of Chemical Theory and Computation, 2012, 8, 3384-3394. | 5.3 | 39 |
| 40 | RESPAC: Method to Determine Partial Charges in Coarse-Grained Protein Model and Its Application to DNA-Binding Proteins. Journal of Chemical Theory and Computation, 2014, 10, 711-721. | 5.3 | 39 |
| 41 | Chromatin remodelers couple inchworm motion with twist-defect formation to slide nucleosomal DNA. PLoS Computational Biology, 2018, 14, e1006512. | 3.2 | 39 |
| 42 | Competition between Protein Folding and Aggregation with Molecular Chaperones in Crowded Solutions: Insight from Mesoscopic Simulations. Biophysical Journal, 2003, 85, 3521-3531. | 0.5 | 38 |
| 43 | Flexible Fitting of Biomolecular Structures to Atomic Force Microscopy Images via Biased Molecular Simulations. Journal of Chemical Theory and Computation, 2020, 16, 1349-1358. | 5.3 | 38 |
| 44 | Structural Comparison of F1-ATPase: Interplay among Enzyme Structures, Catalysis, and Rotations. Structure, 2011, 19, 588-598. | 3.3 | 36 |
| 45 | Protein Grabs a Ligand by Extending Anchor Residues: Molecular Simulation for Ca2+ Binding to Calmodulin Loop. Biophysical Journal, 2006, 90, 3043-3051. | 0.5 | 34 |
| 46 | Molecular dynamics simulation of proton-transfer coupled rotations in ATP synthase FO motor. Scientific Reports, 2020, 10, 8225. | 3.3 | 34 |
| 47 | Secondary structure provides a template for the folding of nearby polypeptides. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 17765-17770. | 7.1 | 31 |
| 48 | Histone acetylation dependent energy landscapes in tri-nucleosome revealed by residue-resolved molecular simulations. Scientific Reports, 2016, 6, 34441. | 3.3 | 31 |
| 49 | Statics, metastable states, and barriers in protein folding: A replica variational approach. Physical Review E, 1997, 55, 4562-4577. | 2.1 | 30 |
| 50 | p53 dynamics upon response element recognition explored by molecular simulations. Scientific Reports, 2015, 5, 17107. | 3.3 | 30 |
| 51 | Role of bacterial RNA polymerase gate opening dynamics in DNA loading and antibiotics inhibition elucidated by quasi-Markov State Model. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, . | 7.1 | 30 |
| 52 | Paddling mechanism for the substrate translocation by AAA+ motor revealed by multiscale molecular simulations. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 18237-18242. | 7.1 | 29 |
| 53 | Allosteric conformational change cascade in cytoplasmic dynein revealed by structure-based molecular simulations. PLoS Computational Biology, 2017, 13, e1005748. | 3.2 | 29 |
| 54 | Multi-scale Ensemble Modeling of Modular Proteins with Intrinsically Disordered Linker Regions: Application to p53. Biophysical Journal, 2014, 107, 721-729. | 0.5 | 28 |

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| 56 | Reconstruction of Atomistic Structures from Coarse-Grained Models for Protein–DNA Complexes. Journal of Chemical Theory and Computation, 2018, 14, 1682-1694. | 5.3 | 27 |
| 57 | Dynamic and Structural Modeling of the Specificity in Protein–DNA Interactions Guided by Binding Assay and Structure Data. Journal of Chemical Theory and Computation, 2018, 14, 3877-3889. | 5.3 | 27 |
| 58 | Implementation of residue-level coarse-grained models in GENESIS for large-scale molecular dynamics simulations. PLoS Computational Biology, 2022, 18, e1009578. | 3.2 | 27 |
| 59 | Microscopic theory of critical folding nuclei and reconfiguration activation barriers in folding proteins. Journal of Chemical Physics, 1997, 107, 9585-9598. | 3.0 | 26 |
| 60 | Multidimensional tunneling in terms of complex classical mechanics: Wave functions, energy splittings, and decay rates in nonintegrable systems. Journal of Chemical Physics, 1996, 104, 3742-3759. | 3.0 | 25 |
| 61 | Overcoming the Bottleneck of the Enzymatic Cycle by Steric Frustration. Physical Review Letters, 2019, 122, 238102. | 7.8 | 24 |
| 62 | How Co-translational Folding of Multi-domain Protein Is Affected by Elongation Schedule: Molecular Simulations. PLoS Computational Biology, 2015, 11, e1004356. | 3.2 | 22 |
| 63 | Self-learning multiscale simulation for achieving high accuracy and high efficiency simultaneously. Journal of Chemical Physics, 2009, 130, 214108. | 3.0 | 19 |
| 64 | The kinetic landscape of nucleosome assembly: A coarse-grained molecular dynamics study. PLoS Computational Biology, 2021, 17, e1009253. | 3.2 | 19 |
| 65 | Reaction dynamics of D+H2â†'DH+H: Effects of potential energy surface topography and usefulness of the constant centrifugal potential approximation. Journal of Chemical Physics, 1992, 96, 339-348. | 3.0 | 18 |
| 66 | Protein folding mechanisms and energy landscape of src SH3 domain studied by a structure prediction toolbox. Chemical Physics, 2004, 307, 157-162. | 1.9 | 18 |
| 67 | Characterizing Protein Energy Landscape by Self-Learning Multiscale Simulations: Application to a Designed β-Hairpin. Biophysical Journal, 2010, 99, 3029-3037. | 0.5 | 17 |
| 68 | Couplings between hierarchical conformational dynamics from multi-time correlation functions and two-dimensional lifetime spectra: Application to adenylate kinase. Journal of Chemical Physics, 2015, 142, 212404. | 3.0 | 17 |
| 69 | Nucleosome Crowding in Chromatin Slows the Diffusion but Can Promote Target Search of Proteins. Biophysical Journal, 2019, 116, 2285-2295. | 0.5 | 17 |
| 70 | Roles of physical interactions in determining protein-folding mechanisms: Molecular simulation of protein G and \hat{l}_{\pm} spectrin SH3. Proteins: Structure, Function and Bioinformatics, 2004, 55, 128-138. | 2.6 | 16 |
| 71 | Dimer domain swapping versus monomer folding in apo-myoglobin studied by molecular simulations. Physical Chemistry Chemical Physics, 2015, 17, 5006-5013. | 2.8 | 16 |
| 72 | Proteinâ€specific force field derived from the fragment molecular orbital method can improve protein–ligand binding interactions. Journal of Computational Chemistry, 2013, 34, 1251-1257. | 3.3 | 15 |

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| 73 | Structure-based Molecular Simulations Reveal the Enhancement of Biased Brownian Motions in Single-headed Kinesin. PLoS Computational Biology, 2013, 9, e1002907. | 3.2 | 15 |
| 74 | On the ATP binding site of the $\hat{l}\mu$ subunit from bacterial F-type ATP synthases. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 332-340. | 1.0 | 14 |
| 75 | Nucleosomes as allosteric scaffolds for genetic regulation. Current Opinion in Structural Biology, 2020, 62, 93-101. | 5.7 | 14 |
| 76 | The HMGB chromatin protein Nhp6A can bypass obstacles when traveling on DNA. Nucleic Acids Research, 2020, 48, 10820-10831. | 14.5 | 14 |
| 77 | Rigid-body fitting to atomic force microscopy images for inferring probe shape and biomolecular structure. PLoS Computational Biology, 2021, 17, e1009215. | 3.2 | 14 |
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| 79 | The structural basis of a high affinity ATP binding ε subunit from a bacterial ATP synthase. PLoS ONE, 2017, 12, e0177907. | 2.5 | 13 |
| 80 | Particle Filter Method to Integrate High-Speed Atomic Force Microscopy Measurements with Biomolecular Simulations. Journal of Chemical Theory and Computation, 2020, 16, 6609-6619. | 5. 3 | 12 |
| 81 | Opening of cohesin's SMC ring is essential for timely DNA replication and DNA loop formation. Cell Reports, 2021, 35, 108999. | 6.4 | 12 |
| 82 | Testing mechanisms of DNA sliding by architectural DNA-binding proteins: dynamics of single wild-type and mutant protein molecules <i>in vitro</i> and <i>in vivo</i> Nucleic Acids Research, 2021, 49, 8642-8664. | 14.5 | 11 |
| 83 | Case Report: Bayesian Statistical Inference of Experimental Parameters via Biomolecular Simulations: Atomic Force Microscopy. Frontiers in Molecular Biosciences, 2021, 8, 636940. | 3.5 | 10 |
| 84 | Folding Coupled with Assembly in Split Green Fluorescent Proteins Studied by Structure-based Molecular Simulations. Journal of Physical Chemistry B, 2013, 117, 13212-13218. | 2.6 | 9 |
| 85 | On the Mg2+ binding site of the ε subunit from bacterial F-type ATP synthases. Biochimica Et Biophysica Acta - Bioenergetics, 2015, 1847, 1101-1112. | 1.0 | 9 |
| 86 | Resolving the data asynchronicity in high-speed atomic force microscopy measurement via the Kalman Smoother. Scientific Reports, 2020, 10, 18393. | 3.3 | 9 |
| 87 | Linker DNA Length is a Key to Tri-nucleosome Folding. Journal of Molecular Biology, 2021, 433, 166792. | 4.2 | 8 |
| 88 | Constant centrifugal potential approximation for atom–diatom chemical reaction dynamics. Journal of Chemical Physics, 1994, 100, 4284-4293. | 3.0 | 7 |
| 89 | How one-dimensional diffusion of transcription factors are affected by obstacles: coarse-grained molecular dynamics study. Molecular Simulation, 2017, 43, 1315-1321. | 2.0 | 7 |
| 90 | Coarse-grained implicit solvent lipid force field with a compatible resolution to the Cα protein representation. Journal of Chemical Physics, 2020, 153, 205101. | 3.0 | 7 |

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| 91 | Rotational Mechanism of FO Motor in the F-Type ATP Synthase Driven by the Proton Motive Force. Frontiers in Microbiology, 0, 13 , . | 3.5 | 6 |
| 92 | The lane-switch mechanism for nucleosome repositioning by DNA translocase. Nucleic Acids Research, 2021, 49, 9066-9076. | 14.5 | 5 |
| 93 | Bayesian Parameter Inference by Markov Chain Monte Carlo with Hybrid Fitness Measures: Theory and Test in Apoptosis Signal Transduction Network. PLoS ONE, 2013, 8, e74178. | 2.5 | 5 |
| 94 | Asymmetry in Membrane Protein Sequence and Structure: Glycine Outside Rule. Journal of Molecular Biology, 2008, 377, 74-82. | 4.2 | 4 |
| 95 | Rigor of cell fate decision by variable p53 pulses and roles of cooperative gene expression by p53. Biophysics (Nagoya-shi, Japan), 2012, 8, 41-50. | 0.4 | 4 |
| 96 | How Cytoplasmic Dynein Couples ATP Hydrolysis Cycle to Diverse Stepping Motions: Kinetic Modeling. Biophysical Journal, 2020, 118, 1930-1945. | 0.5 | 4 |
| 97 | Modeling of DNA binding to the condensin hinge domain using molecular dynamics simulations guided by atomic force microscopy. PLoS Computational Biology, 2021, 17, e1009265. | 3.2 | 4 |
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| 99 | Cooperation among c-subunits of FoF1-ATP synthase in rotation-coupled proton translocation. ELife, 2022, 11, . | 6.0 | 4 |
| 100 | Inferring Conformational State of Myosin Motor in an Atomic Force Microscopy Image via Flexible Fitting Molecular Simulations. Frontiers in Molecular Biosciences, 2022, 9, 882989. | 3.5 | 4 |
| 101 | In Silico Chaperonin-Like Cycle Helps Folding of Proteins for Structure Prediction. Biophysical Journal, 2008, 94, 2558-2565. | 0.5 | 3 |
| 102 | Modeling lipid–protein interactions for coarse-grained lipid and Cα protein models. Journal of Chemical Physics, 2021, 155, 155101. | 3.0 | 3 |
| 103 | WKB Theory of Tunneling between Tori. Progress of Theoretical Physics Supplement, 1994, 116, 295-301. | 0.1 | 3 |
| 104 | Simulating Folding of Helical Proteins with Coarse Grained Models. Progress of Theoretical Physics Supplement, 2000, 138, 366-371. | 0.1 | 2 |
| 105 | Semi-Implicit Time Integration with Hessian Eigenvalue Corrections for a Larger Time Step in Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2021, 17, 5792-5804. | 5.3 | 2 |
| 106 | Glassy Dynamics of Random Heteropolymers. Progress of Theoretical Physics Supplement, 1997, 126, 49-52. | 0.1 | 2 |
| 107 | Coarse-grained molecular dynamics simulations of base-pair mismatch recognition protein MutS sliding along DNA. Biophysics and Physicobiology, 2022, 19, . | 1.0 | 2 |
| 108 | Molecular Mechanism of Allostery: MWC or KNF Model?-Approach by Theoretical Model Calculation. Seibutsu Butsuri, 2009, 49, 132-134. | 0.1 | 1 |

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| 109 | 35 Years of the Go Model. Seibutsu Butsuri, 2010, 50, 158-159. | 0.1 | 1 |
| 110 | Applying a grid technology to protein structure predictor "ROKKY". Studies in Health Technology and Informatics, 2005, 112, 27-36. | 0.3 | 1 |
| 111 | Using incomplete Cholesky factorization to increase the time step in molecular dynamics simulations. Journal of Computational and Applied Mathematics, 2022, 415, 114519. | 2.0 | 1 |
| 112 | S09A4 Rotary mechanisms of F1-ATPase revealed by molecular simulations(Mechanism of F_1-ATPase) Tj ETQq0 0 | 0 0 rgBT /O | Overlock 10 T O |
| 113 | 1P-145 Simulation study on stepping mechanism of Conventional Kinesin by coarse-grained model(The) Tj ETQq1 | 1 ₀ .178431 | .4 rgBT /Ove |
| 114 | 1P-065 Simulating large-scale conformational change in a virus protein that mediates membrane fusion(The 46th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2008, 48, S31. | 0.1 | 0 |
| 115 | 2S4-4 Structure change coupled with binding and its application to biomolecular systems(2S4 What) Tj ETQq1 1 (Seibutsu Butsuri, 2008, 48, S10. | 0.784314 r 0.1 | rgBT /Overlo |
| 116 | 3P-182 Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation(Biol & Artifi memb.:Dynamics,Oral Presentations,The 47th Annual Meeting of the) Tj ETQq0 0 0 rgBT /C | Ovædlock 10 | OoTf 50 457 |
| 117 | 1TP5-07 Coarse-grained simulation of protein-DNA complex : dynamics of nucleosome(The 47th Annual) Tj ETQq1 | 1.9.7843 | 14 rgBT /0v |
| 118 | 1P-099 Coarse-grained simulation of protein-DNA complex: dynamics of nucleosome (Nucleic) Tj ETQq0 0 0 rgBT / Seibutsu Butsuri, 2009, 49, S79. | /Overlock 1 0.1 | 10 Tf 50 387 0 |
| 119 | 2P-002 Folding simulations of chignolin by self-learning multiscale method(Protein:Structure, The) Tj ETQq1 1 0.78 | 84314 rgB | T/Overlock |
| 120 | 1TA4-02 Mechanism of unidirectional move of KIF1A motor studied by coarse-grained simulations(The) Tj ETQq0 C |) 8.fgBT /C | Overlock 10 |
| 121 | 2TP5-02 Folding simulations of chignolin by self-learning multiscale method(The 47th Annual Meeting) Tj ETQq1 1 | 0.784314 0.1 | 4 rgBT /Over |
| 122 | 3TA3-02 Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation(The 47th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2009, 49, S54-S55. | 0.1 | 0 |
| 123 | 1P-129 Mechanism of unidirectional move of KIF1A motor studied by coarse-grained simulations(Molecular motor, The 47th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2009, 49, S83. | 0.1 | 0 |
| 124 | 3P-183 Membrane morphology dynamics induced by proteins: Coarsegrained molecular simulations(Biol & Coarsegrained Society of) Tj ETQq0 0 | OorgBT /O | v e rlock 10 T |
| 125 | 1P-098 Replica exchange simulations applied for coarse-grained models of giant protein-nucleic acid complex(Nucleic acid:Interaction & ETQq1 1 0.78431) | l∳ngBT/O | verlock 10 T |
| 126 | 1P136 Coarse-grained simulation of protein-DNA complex : mechanical unzipping of nucleosome(Nucleic acid:Interaction & Complex formation,The 48th Annual Meeting of the Biophysical) Tj ETQq0 | 0001rgBT / | Overlock 10 |

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| 127 | 2P119 Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation(The 48th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2010, 50, S103. | 0.1 | O |
| 128 | 3P309 Modeling Rhodopsin active conformation (Meta II) by molecular dynamics simulations(Mathematical biology,The 48th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2010, 50, S200. | 0.1 | 0 |
| 129 | 3A1112 Molecular dynamics simulation of pH-activated KcsA channel(3A Biol & Samp; Artifi memb 3:) Tj ETQq1 1 CButsuri, 2011, 51, S105. | 0.784314 rg 0.1 | gBT /Overloo 0 |
| 130 | 1C1436 Coarse-grained simulations of multi-nucleosome systems(Nucleic acid,The 49th Annual Meeting) Tj ETQo | 000 rgB1 | 「 Overlock] |
| 131 | 1Q1324 Activation mechanism of rhodopsin elucidated by molecular dynamics simulations(Photobiology: Vision & Dynamics 1,The 49th Annual Meeting of the Biophysical) Tj ETQq1 | 1 @.7 8431 | .40rgBT /Ove |
| 132 | 3PT009 Mono- and poly-nucleosome structural dynamics by coarse-grained simulations(The 50th) Tj ETQq0 0 0 r | gBT /Overlo | ock 10 Tf 50 |
| 133 | 3PT011 Diffusion of TFIIIA zinc fingers along DNA studied by molecular simulations(The 50th Annual) Tj ETQq1 $$ 1 | 0.784314 | rgBT /Overio |
| 134 | 1P149 The Mg^<2+> binding site of the ATP synthase $\hat{l}\mu$ subunit from Bacillus subtilis derived by Molecular Dynamics simulations(11.Molecular motor,Poster,The 51st Annual Meeting of the) Tj ETQq0 0 0 rgBT / | O vet lock 1 | .0oTf 50 457 |
| 135 | 3P121 Poly-nucleosome structural dynamics by coarse-grained simulations(05A. Nucleic acid:) Tj ETQq1 1 0.7843 | 314 rgBT /C | Dverlock 10 |
| 136 | 2SCP-03 Structure of model chromatin and dynamics of transcription factors studied by coarse-grained simulations(2SCP Functional dynamics of Nucleosome and Chromathin in Nuclear) Tj ETQq0 0 0 r | gBT ∫Overlo 0.1 | ock 10 Tf 50 |
| 137 | Seibutsu Butsuri, 2013, 53, S98. Molecular Dynamics Simulations of Biomolecules. Journal of the Society of Mechanical Engineers, 2013, 116, 78-80. | 0.0 | 0 |
| 138 | 1P148 Molecular mechanism of the epsilon subunit from F-type ATP synthases studied by Molecular Dynamics simulations(11. Molecular motor,Poster,The 52nd Annual Meeting of the Biophysical Society) Tj ETQqC | 0001rgBT / | Overlock 10 |
| 139 | 3P276 Comprehensive analysis of protein folding energy landscape by multicanonical Go-model molecular dynamics simulation(24. Mathematical biology,Poster,The 52nd Annual Meeting of the) Tj ETQq1 1 0.7 | '8 ⊕3 14 rgE | 3Td/Overlock |

Coarse-grained Biomolecular Simulations. Seibutsu Butsuri, 2021, 61, 144-151.

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