Ryuhei Harada

List of Publications by Year
in descending order

62	798	471509 17	552781 26
papers	citations	h-index	g-index

63	63	63	349
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Parallel cascade selection molecular dynamics (PaCS-MD) to generate conformational transition pathway. Journal of Chemical Physics, 2013, 139, 035103.	3.0	110
2	Simple, yet powerful methodologies for conformational sampling of proteins. Physical Chemistry Chemical Physics, 2015, 17, 6155-6173.	2.8	55
3	Exploring the Folding Free Energy Landscape of a Î²-Hairpin Miniprotein, Chignolin, Using Multiscale Free Energy Landscape Calculation Method. Journal of Physical Chemistry B, 2011, 115, 8806-8812.	2.6	45
4	Nontargeted Parallel Cascade Selection Molecular Dynamics for Enhancing the Conformational Sampling of Proteins. Journal of Chemical Theory and Computation, 2015, 11, 5493-5502.	5.3	41
5	Identification of the key interactions in structural transition pathway of FtsZ from Staphylococcus aureus. Journal of Structural Biology, 2017, 198, 65-73.	2.8	41
6	Protein folding pathways extracted by OFLOOD: Outlier FLOODing method. Journal of Computational Chemistry, 2015, 36, 97-102.	3.3	30
7	Efficient Conformational Search Based on Structural Dissimilarity Sampling: Applications for Reproducing Structural Transitions of Proteins. Journal of Chemical Theory and Computation, 2017, 13, 1411-1423.	5.3	26
8	Fluctuation Flooding Method (FFM) for accelerating conformational transitions of proteins. Journal of Chemical Physics, 2014, 140, 125103.	3.0	25
9	Simple, yet Efficient Conformational Sampling Methods for Reproducing/Predicting Biologically Rare Events of Proteins. Bulletin of the Chemical Society of Japan, 2018, 91, 1436-1450.	3.2	25
10	On the inducedâ€fit mechanism of substrateâ€enzyme binding structures of nylonâ€oligomer hydrolase. Journal of Computational Chemistry, 2014, 35, 1240-1247.	3.3	23
11	Temperatureâ€shuffled parallel cascade selection molecular dynamics accelerates the structural transitions of proteins. Journal of Computational Chemistry, 2017, 38, 2671-2674.	3.3	23
12	The Fast-Folding Mechanism of Villin Headpiece Subdomain Studied by Multiscale Distributed Computing. Journal of Chemical Theory and Computation, 2012, 8, 290-299.	5.3	22
13	Parallel cascade selection molecular dynamics for efficient conformational sampling and free energy calculation of proteins. AIP Conference Proceedings, 2016, , .	0.4	22
14	Enhanced conformational sampling method for proteins based on the <scp>T</scp>a<scp>B</scp>oo <scp>S</scp>e<scp>A</scp>rch algorithm: Application to the folding of a miniâ€protein, chignolin. Journal of Computational Chemistry, 2015, 36, 763-772.	3.3	20
15	Sparsityâ€weighted outlier <scp>FLOOD</scp>ing (<scp>OFLOOD</scp>) method: Efficient rare event sampling method using sparsity of distribution. Journal of Computational Chemistry, 2016, 37, 724-738.	3.3	20
16	A Fast Convergent Simulated Annealing Algorithm for Protein-Folding: Simulated Annealing Outlier FLOODing (SA-OFLOOD) Method. Bulletin of the Chemical Society of Japan, 2016, 89, 1361-1367.	3.2	19
17	Automatic detection of hidden dimensions to obtain appropriate reaction coordinates in the Outlier FLOODing (OFLOOD) method. Chemical Physics Letters, 2015, 639, 269-274.	2.6	17
18	Nontargeted Parallel Cascade Selection Molecular Dynamics Using Time-Localized Prediction of Conformational Transitions in Protein Dynamics. Journal of Chemical Theory and Computation, 2019, 15, 5144-5153.	5.3	12

#	Article	IF	Citations
19	Hybrid Cascade-Type Molecular Dynamics with a Markov State Model for Efficient Free Energy Calculations. Journal of Chemical Theory and Computation, 2019, 15, 680-687.	5.3	12
20	Structural dissimilarity sampling with dynamically self-guiding selection. Journal of Computational Chemistry, 2017, 38, 1921-1929.	3.3	11
21	The role of <scp>ATP</scp> in solubilizing <scp>RNA</scp>â€binding protein fused in sarcoma. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1606-1612.	2.6	11
22	Multi-Scale Free Energy Landscape calculation method by combination of coarse-grained and all-atom models. Chemical Physics Letters, 2011, 503, 145-152.	2.6	10
23	Common folding processes of mini-proteins: Partial formations of secondary structures initiate the immediate protein folding. Journal of Computational Chemistry, 2017, 38, 790-797.	3.3	10
24	Efficient Conformational Sampling of Collective Motions of Proteins with Principal Component Analysis-Based Parallel Cascade Selection Molecular Dynamics. Journal of Chemical Information and Modeling, 2020, 60, 4021-4029.	5.4	10
25	pyProGAâ€”A PyMOL plugin for protein residue network analysis. PLoS ONE, 2021, 16, e0255167.	2.5	10
26	Efficient conformational sampling of proteins based on a multi-dimensional TaBoo SeArch algorithm: An application to folding of chignolin in explicit solvent. Chemical Physics Letters, 2015, 630, 68-75.	2.6	9
27	TaBoo SeArch Algorithm with a Modified Inverse Histogram for Reproducing Biologically Relevant Rare Events of Proteins. Journal of Chemical Theory and Computation, 2016, 12, 2436-2445.	5.3	9
28	On-the-Fly Specifications of Reaction Coordinates in Parallel Cascade Selection Molecular Dynamics Accelerate Conformational Transitions of Proteins. Journal of Chemical Theory and Computation, 2018, 14, 3332-3341.	5.3	9
29	Temperature-Shuffled Structural Dissimilarity Sampling Based on a Root-Mean-Square Deviation. Journal of Chemical Information and Modeling, 2018, 58, 1397-1405.	5.4	9
30	How Does the Number of Initial Structures Affect the Conformational Sampling Efficiency and Quality in Parallel Cascade Selection Molecular Dynamics (PaCS-MD)?. Chemistry Letters, 2017, 46, 862-865.	1.3	8
31	Dynamic Specification of Initial Structures in Parallel Cascade Selection Molecular Dynamics (PaCS-MD) Efficiently Promotes Biologically Relevant Rare Events. Bulletin of the Chemical Society of Japan, 2017, 90, 1236-1243.	3.2	8
32	Self-Avoiding Conformational Sampling Based on Histories of Past Conformational Searches. Journal of Chemical Information and Modeling, 2017, 57, 3070-3078.	5.4	7
33	Programed dynamical ordering in self-organization processes of a nanocube: a molecular dynamics study. Physical Chemistry Chemical Physics, 2018, 20, 9115-9122.	2.8	7
34	Conformational transition pathway and free energy analyses of proteins by parallel cascade selection molecular dynamics (PaCS-MD). AIP Conference Proceedings, 2014, , .	0.4	6
35	Molecular mechanisms of substrate specificities of uridine-cytidine kinase. Biophysics and Physicobiology, 2016, 13, 77-84.	1.0	6
36	An assessment of optimal time scale of conformational resampling for parallel cascade selection molecular dynamics. Molecular Simulation, 2018, 44, 206-212.	2.0	6

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37	Quantal cumulant dynamics for realâ€time simulations of quantum manyâ€body systems. International Journal of Quantum Chemistry, 2015, 115, 300-308.	2.0	5
38	Nontargeted Parallel Cascade Selection Molecular Dynamics Based on a Nonredundant Selection Rule for Initial Structures Enhances Conformational Sampling of Proteins. Journal of Chemical Information and Modeling, 2019, 59, 5198-5206.	5.4	5
39	Protein Dynamics and the Folding Degree. Journal of Chemical Information and Modeling, 2020, 60, 1559-1567.	5.4	5
40	Temperatureâ€“pressure shuffling outlier flooding method enhances the conformational sampling of proteins. Journal of Computational Chemistry, 2019, 40, 1530-1537.	3.3	4
41	Molecular Mechanism of the Reaction Specificity in Threonine Synthase: Importance of the Substrate Conformations. Journal of Physical Chemistry B, 2017, 121, 5536-5543.	2.6	3
42	Selection rules on initial structures in parallel cascade selection molecular dynamics affect conformational sampling efficiency. Journal of Molecular Graphics and Modelling, 2018, 85, 153-159.	2.4	3
43	How low-resolution structural data predict the conformational changes of a protein: a study on data-driven molecular dynamics simulations. Physical Chemistry Chemical Physics, 2018, 20, 17790-17798.	2.8	3
44	Molecular Mechanism for the Actin-Binding Domain of Î±-Actinin Ain1 Elucidated by Molecular Dynamics Simulations and Mutagenesis Experiments. Journal of Physical Chemistry B, 2020, 124, 8495-8503.	2.6	3
45	The Folding of Trp-cage is Regulated by Stochastic Flip of the Side Chain of Tryptophan. Chemistry Letters, 2021, 50, 162-165.	1.3	3
46	Residue Folding Degreeâ€”Relationship to Secondary Structure Categories and Use as Collective Variable. International Journal of Molecular Sciences, 2021, 22, 13042.	4.1	3
47	Selection Rules for Outliers in Outlier Flooding Method Regulate Its Conformational Sampling Efficiency. Journal of Chemical Information and Modeling, 2019, 59, 3919-3926.	5.4	2
48	Enhanced Conformational Sampling Method Based on Anomaly Detection Parallel Cascade Selection Molecular Dynamics: ad-PaCS-MD. Journal of Chemical Theory and Computation, 2020, 16, 6716-6725.	5.3	2
49	Independent Nontargeted Parallel Cascade Selection Molecular Dynamics (Ino-PaCS-MD) to Enhance the Conformational Sampling of Proteins. Journal of Chemical Theory and Computation, 2021, 17, 5933-5943.	5.3	2
50	Phosphorylation in the accessory domain of yeast histone chaperone protein 1 exposes the nuclear export signal sequence. Proteins: Structure, Function and Bioinformatics, 2022, 90, 317-321.	2.6	2
51	A post-process to estimate an approximated minimal free energy path based on local centroids. Chemical Physics Letters, 2021, 782, 139003.	2.6	2
52	Structural Validation by the G-Factor Properly Regulates Boost Potentials Imposed in Conformational Sampling of Proteins. Journal of Chemical Information and Modeling, 2022, 62, 3442-3452.	5.4	2
53	How Does Friction Coefficient Affect the Conformational Sampling Efficiency of Parallel Cascade Selection Molecular Dynamics?. Chemistry Letters, 2018, 47, 1119-1122.	1.3	1
54	Parallel cascade selection molecular dynamics to screen for protein complexes generated by rigid docking. Journal of Molecular Graphics and Modelling, 2019, 92, 94-99.	2.4	1

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55	Comprehensive predictions of secondary structures for comparative analysis in different species. Journal of Structural Biology, 2021, 213, 107735.	2.8	1
56	Rearrangements of Water Molecules in Parallel Cascade Selection Molecular Dynamics Enhance Structural Explorations of Proteins. Bulletin of the Chemical Society of Japan, 2021, 94, 97-105.	3.2	1
57	Structural Variations of Metallothionein with or without Zinc Ions Elucidated by All-Atom Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2021, 125, 12712-12717.	2.6	1
58	Histone H3 Inhibits Ubiquitin-Ubiquitin Intermolecular Interactions to Enhance Binding to DNA Methyl Transferase 1. Journal of Molecular Biology, 2022, 434, 167371.	4.2	1
59	Ligand Binding Path Sampling Based on Parallel Cascade Selection Molecular Dynamics: LB-PaCS-MD. Materials, 2022, 15, 1490.	2.9	1
60	Parallel Cascade Selection Molecular Dynamics Simulations for Transition Pathway Sampling of Biomolecules. Advances in Quantum Chemistry, 2019, , 129-147.	0.8	0
61	In silico mutational analyses reveal different ligand-binding abilities of double pockets of medaka fish taste receptor type 1 essential for efficient taste recognition. Physical Chemistry Chemical Physics, 2021, 23, 20398-20405.	2.8	0
62	Analyses on Dynamical Ordering of Protein Functions by Means of Cascade Selection Molecular Dynamics. Journal of Computer Chemistry Japan, 2018, 17, 46-56.	0.1	0