Yasuteru Shigeta

List of Publications by Year
in descending order

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321 papers	5,440 citations	136950 32 h-index	123424 61 g-index
328 all docs	328 docs citations	328 times ranked	5427 citing authors

#	Article	IF	Citations
1	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
2	Next generation quantum theory of atoms in molecules for the design of emitters exhibiting thermally activated delayed fluorescence with laser irradiation. Journal of Computational Chemistry, 2022, 43, 206-214.	3.3	4
3	Ligand Binding Path Sampling Based on Parallel Cascade Selection Molecular Dynamics: LB-PaCS-MD. Materials, 2022, 15, 1490.	2.9	1
4	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
5	Halogenated Baicalein as a Promising Antiviral Agent toward SARS-CoV-2 Main Protease. Journal of Chemical Information and Modeling, 2022, 62, 1498-1509.	5.4	30
6	Semi-Synthesis of N-Aryl Amide Analogs of Piperine from Piper nigrum and Evaluation of Their Antitrypanosomal, Antimalarial, and Anti-SARS-CoV-2 Main Protease Activities. Molecules, 2022, 27, 2841.	3.8	10
7	Evaluation of an Appropriate Standard Hydrogen Electrode Potential for Computing Redox Potentials of Catechins with Density Functional Theory. Chemistry Letters, 2022, 51, 673-677.	1.3	0
8	Heme-bound tyrosine vibrations in hemoglobin M: Resonance Raman, crystallography, and DFT calculation. Biophysical Journal, 2022, 121, 2767-2780.	0.5	3
9	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
10	Conformation-Changeable Ï€-Electronic Systems with Metastable Bent-Core Conformations and Liquid-Crystalline-State Electric-Field-Responsive Properties. Organic Letters, 2021, 23, 305-310.	4.6	4
11	Ion-pairing Ï€-electronic systems: ordered arrangement and noncovalent interactions of negatively charged porphyrins. Chemical Science, 2021, 12, 9645-9657.	7.4	23
12	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
13	Interaction of 8-anilinonaphthalene-1-sulfonate with SARS-CoV-2 main protease and its application as a fluorescent probe for inhibitor identification. Computational and Structural Biotechnology Journal, 2021, 19, 3364-3371.	4.1	26
14	Molecular Motions of Imidazole in Poly(vinylphosphonic acid)-Imidazole Composites Investigated by Molecular Dynamics Simulations. Chemistry Letters, 2021, 50, 17-20.	1.3	4
15	AnalysisFMO Toolkit: A PyMOL Plugin for 3D-Visualization of Interaction Energies in Proteins (3D-VIEP) Calculated by the FMO Method. , 2021, , 357-370.		0
16	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
17	Estimation of the relative contributions to the electronic energy transfer rates based on FÃ¶rster theory: The case of C-phycocyanin chromophores. Biophysics and Physicobiology, 2021, 18, 196-214.	1.0	3
18	Linear Combination of Molecular Orbitals of Fragments (FMO-LCMO) Method: Its Application to Charge Transfer Studies. , 2021, , 391-405.		1

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19	Computational Analysis Reveals a Critical Point Mutation in the N-Terminal Region of the Signaling Lymphocytic Activation Molecule Responsible for the Cross-Species Infection with Canine Distemper Virus. Molecules, 2021, 26, 1262.	3.8	4
20	Split conformation of Chaetomium thermophilum Hsp104 disaggregase. Structure, 2021, 29, 721-730.e6.	3.3	2
21	Comparison between the Light-Harvesting Mechanisms of Type-I Photosynthetic Reaction Centers of Heliobacteria and Photosystem I: Pigment Site Energy Distribution and Exciton State. Journal of Physical Chemistry B, 2021, 125, 3727-3738.	2.6	5
22	Weak O2 binding and strong H2O2 binding at the non-heme diiron center of trypanosome alternative oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2021, 1862, 148356.	1.0	7
23	Structure, solubility, and permeability relationships in a diverse middle molecule library. Bioorganic and Medicinal Chemistry Letters, 2021, 37, 127847.	2.2	3
24	Proton Conduction Mechanism for Anhydrous Imidazolium Hydrogen Succinate Based on Local Structures and Molecular Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 5390-5394.	4.6	18
25	pyProGAâ€"A PyMOL plugin for protein residue network analysis. PLoS ONE, 2021, 16, e0255167.	2.5	10
26	On-Demand Chirality Transfer of Human Serum Albumin to Bis(thiophen-2-yl)hexafluorocyclopentenes through Their Photochromic Ring Closure. Journal of Organic Chemistry, 2021, 86, 12549-12558.	3.2	8
27	A Practical Prediction of LogPo/w through Semiempirical Electronic Structure Calculations with Dielectric Continuum Model. Bulletin of the Chemical Society of Japan, 2021, 94, 1807-1814.	3.2	3
28	Could London Dispersion Force Control Regioselective (2 + 2) Cyclodimerizations of Benzynes? YES: Application to the Synthesis of Helical Biphenylenes. Journal of the American Chemical Society, 2021, 143, 10853-10859.	13.7	19
29	Control of chirality, bond flexing and anharmonicity in an electric field. International Journal of Quantum Chemistry, 2021, 121, e26793.	2.0	8
30	Solvophobicity-directed assembly of microporous molecular crystals. Communications Chemistry, 2021, 4, .	4.5	7
31	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
32	Chirality without Stereoisomers: Insight fromÂthe Helical Response of Bond Electrons. ChemPhysChem, 2021, 22, 1989-1995.	2.1	8
33	Solubility and Membrane Permeability of Cyclic Dipeptides Approximately Estimated by Quantum Chemistry and Molecular Dynamics Calculations. Chemistry Letters, 2021, 50, 1964-1967.	1.3	1
34	A post-process to estimate an approximated minimal free energy path based on local centroids. Chemical Physics Letters, 2021, 782, 139003.	2.6	2
35	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
36	Structural and functional characterization of nylon hydrolases. Methods in Enzymology, 2021, 648, 357-389.	1.0	8

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37	Effects of mechanical grinding on the phase behavior and anhydrous proton conductivity of imidazolium hydrogen succinate. Solid State Ionics, 2021, 372, 115775.	2.7	4
38	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
39	Alkyne-Tagged Apigenin, a Chemical Tool to Navigate Potential Targets of Flavonoid Anti-Dengue Leads. Molecules, 2021, 26, 6967.	3.8	4
40	A Free-Energy Landscape Analysis of Calmodulin Obtained from an NMR Data-Utilized Multi-Scale Divide-and-Conquer Molecular Dynamics Simulation. Life, 2021, 11, 1241.	2.4	0
41	Residue Folding Degreeâ€"Relationship to Secondary Structure Categories and Use as Collective Variable. International Journal of Molecular Sciences, 2021, 22, 13042.	4.1	3
42	Experimental and theoretical study on converting myoglobin into a stable domain-swapped dimer by utilizing a tight hydrogen bond network at the hinge region. RSC Advances, 2021, 11, 37604-37611.	3.6	2
43	Theoretical Prediction of the Redox Potential of Catechins with First Principle Calculation. Journal of Computer Chemistry Japan, 2021, 20, 137-139.	0.1	0
44	Recent Developments of Computational Methods for pKa Prediction Based on Electronic Structure Theory with Solvation Models. J, 2021, 4, 849-864.	0.9	7
45	Multiple Virtual Screening Strategies for the Discovery of Novel Compounds Active Against Dengue Virus: A Hit Identification Study. Scientia Pharmaceutica, 2020, 88, 2.	2.0	24
46	Reaction of threonine synthase with the substrate analogue 2-amino-5-phosphonopentanoate: implications into the proton transfer at the active site. Journal of Biochemistry, 2020, 167, 357-364.	1.7	0
47	Tunneling matrix element and tunneling pathways of protein electron transfer calculated with a fragment molecular orbital method. Journal of Chemical Physics, 2020, 153, 104104.	3.0	2
48	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
49	Self-Associating Curved Ï€-Electronic Systems with Electron-Donating and Hydrogen-Bonding Properties. Journal of the American Chemical Society, 2020, 142, 16420-16428.	13.7	12
50	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
51	Dibromopinocembrin and Dibromopinostrobin Are Potential Anti-Dengue Leads with Mild Animal Toxicity. Molecules, 2020, 25, 4154.	3.8	16
52	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
53	Regenerations of Initial Velocities in Parallel Cascade Selection Molecular Dynamics (PaCS-MD) Enhance the Conformational Transitions of Proteins. Chemistry Letters, 2020, 49, 798-801.	1.3	5
54	Understanding the Detection Mechanisms and Ability of Molecular Hydrogen on Three-Dimensional Bicontinuous Nanoporous Reduced Graphene Oxide. Materials, 2020, 13, 2259.	2.9	0

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55	Neutron crystallography of copper amine oxidase reveals keto/enolate interconversion of the quinone cofactor and unusual proton sharing. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 10818-10824.	7.1	11
56	Analytical Method Using a Scaled Hypersphere Search for High-Dimensional Metadynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 3869-3878.	5.3	7
57	Distribution of Counter Ions in Negatively-charged Lipid/Water/Air Interface: Molecular Dynamics Study. Chemistry Letters, 2020, 49, 361-363.	1.3	1
58	The Dynamics of S-adenosyl-methionine and S-adenosyl-homocysteine in Mouse Dnmt1 is Driven by Their Structural Flexibilities. Chemistry Letters, 2020, 49, 785-788.	1.3	1
59	Protein Dynamics and the Folding Degree. Journal of Chemical Information and Modeling, 2020, 60, 1559-1567.	5.4	5
60	Local Structures and Dynamics of Imidazole Molecules in Poly(vinylphosphonic acid)â€“Imidazole Composite Investigated by Molecular Dynamics. ACS Applied Polymer Materials, 2020, 2, 1561-1568.	4.4	11
61	Intramolecular mode coupling of the isotopomers of water: a non-scalar charge density-derived perspective. Physical Chemistry Chemical Physics, 2020, 22, 2509-2520.	2.8	19
62	Excitonic Coupling on a Heliobacterial Symmetrical Type-I Reaction Center: Comparison with Photosystem I. Journal of Physical Chemistry B, 2020, 124, 389-403.	2.6	8
63	Target Identification Using Homopharma and Network-Based Methods for Predicting Compounds Against Dengue Virus-Infected Cells. Molecules, 2020, 25, 1883.	3.8	4
64	Why Are Lopinavir and Ritonavir Effective against the Newly Emerged Coronavirus 2019? Atomistic Insights into the Inhibitory Mechanisms. Biochemistry, 2020, 59, 1769-1779.	2.5	187
65	Estimation of Acid Dissociation Constants (pK_a) of N-Containing Heterocycles in DMSO and Transferability of Gibbs Free Energy in Different Solvent Conditions. Chemistry Letters, 2020, 49, 307-310.	1.3	5
66	Agonist and Antagonist-Diverted Twisting Motions of a Single TRPV1 Channel. Journal of Physical Chemistry B, 2020, 124, 11617-11624.	2.6	13
67	Reaction mechanism of N-cyclopropylglycine oxidation by monomeric sarcosine oxidase. Physical Chemistry Chemical Physics, 2020, 22, 16552-16561.	2.8	4
68	Unique protonation states of aspartate and topaquinone in the active site of copper amine oxidase. RSC Advances, 2020, 10, 38631-38639.	3.6	8
69	Role of the Propionic Acid Side-Chain of C-Phycocyanin Chromophores in the Excited States for the Photosynthesis Process. Bulletin of the Chemical Society of Japan, 2020, 93, 1509-1519.	3.2	8
70	Photosynergetic Effects on Tripletâ€“Triplet Annihilation Upconversion Processes in Solid Studied by Theory and Experiments. , 2020, , 147-170.		0
71	Numerical investigation of the nano-scale solutal Marangoni convections. Journal of the Taiwan Institute of Chemical Engineers, 2019, 98, 20-26.	5.3	6
72	Parallel Cascade Selection Molecular Dynamics Simulations for Transition Pathway Sampling of Biomolecules. Advances in Quantum Chemistry, 2019, , 129-147.	0.8	0

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73	Accessing the Accuracy of Density Functional Theory through Structure and Dynamics of the Waterâ€“Air Interface. Journal of Physical Chemistry Letters, 2019, 10, 4914-4919.	4.6	43
74	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
75	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
76	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
77	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
78	Possible Configurations of Apo-form Taste Receptor Type 1 (T1r) Studied by Microsecond-order Molecular Dynamics Simulation. Chemistry Letters, 2019, 48, 325-328.	1.3	1
79	Structural Changes of the Trinuclear Copper Center in Bilirubin Oxidase upon Reduction. Molecules, 2019, 24, 76.	3.8	3
80	Quadruply N-methylated octaphyrin: a helical macrocycle exhibiting chiroptical properties and dynamic conformation changes correlated with helical and inner N-methyl orientations. Organic and Biomolecular Chemistry, 2019, 17, 1163-1168.	2.8	8
81	First-Principles Study of the Reaction Mechanism of CHO + H on Graphene Surface. Journal of Physical Chemistry A, 2019, 123, 5633-5639.	2.5	3
82	Elucidation of the entire Kok cycle for photosynthetic water oxidation by the large-scale quantum mechanics/molecular mechanics calculations: Comparison with the experimental results by the recent serial femtosecond crystallography. Chemical Physics Letters, 2019, 730, 416-425.	2.6	8
83	Pyrroleâ€Based Ïâ€Systemâ€“Pt^{II} Complexes: Chiroptical Properties and Excitedâ€State Dynamics with Microsecond Triplet Lifetimes. Chemistry - A European Journal, 2019, 25, 8797-8804.	3.3	6
84	In Silico Structural Modeling and Analysis of Elongation Factor-1 Alpha and Elongation Factor-like Protein. ACS Omega, 2019, 4, 7308-7316.	3.5	5
85	Temperatureâ€“pressure shuffling outlier flooding method enhances the conformational sampling of proteins. Journal of Computational Chemistry, 2019, 40, 1530-1537.	3.3	4
86	Chiralityâ€“Helicity Equivalence in the S and R Stereoisomers: AÂTheoretical Insight. Journal of the American Chemical Society, 2019, 141, 5497-5503.	13.7	29
87	Photosubstitution Reaction of cis-[Ru(bpy)₂(CH₃CN)₂]²⁺ and cis-[Ru(bpy)₂(NH₃)₂]²⁺ in Aqueous Solution via Monoaqua Intermediate. Journal of Physical Chemistry A, 2019, 123, 2497-2502.	2.5	8
88	Reaction mechanism of non-enzymatic stereoselective formation of wine lactone. Chemical Physics Letters, 2019, 725, 114-118.	2.6	0
89	Effects of Antifreezing Protein from Rhagium inquisitor Binding on Ice Growth: A Molecular Dynamics Study. Chemistry Letters, 2019, 48, 223-226.	1.3	0
90	The Study of the Octanol-Water Partition Coefficient by the Computational Chemistry Method. Journal of Computer Chemistry Japan, 2019, 18, 241-243.	0.1	1

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91	New assay method based on Raman spectroscopy for enzymes reacting with gaseous substrates. Protein Science, 2019, 28, 663-670.	7.6	5
92	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
93	Theoretical study of the photodissociation reaction of methanol. Chemical Physics Letters, 2019, 714, 137-142.	2.6	8
94	Development of an Analysis Toolkit, AnalysisFMO, to Visualize Interaction Energies Generated by Fragment Molecular Orbital Calculations. Journal of Chemical Information and Modeling, 2019, 59, 25-30.	5.4	13
95	First-principle study of ammonia decomposition and nitrogen incorporation on the GaN surface in metal organic vapor phase epitaxy. Journal of Crystal Growth, 2019, 507, 421-424.	1.5	6
96	Calculation of Free Energy Reaction Network of Alanine Polypeptide by Using Free Energy Reaction Route Mapping Method. Journal of Computer Chemistry Japan, 2019, 18, 221-223.	0.1	0
97	Developments of Rare Event Sampling Methods for Proteins. Journal of Computer Chemistry Japan, 2019, 18, 199-201.	0.1	0
98	Does Inactive Alkyl Chain Enhance Tripletâ€“Triplet Annihilation of 9,10-Diphenylanthracene Derivatives?. Journal of Physical Chemistry C, 2018, 122, 5334-5340.	3.1	14
99	The effect of octahedral distortions on the electronic properties and magnetic interactions in O3 NaTMO₂ compounds (TM = Tiâ€“Ni & Zrâ€“Pd). RSC Advances, 2018, 8, 13842-13849.	3.6	18
100	Dominant role of orbital splitting in determining cathode potential in O3 NaTMO2 compounds. Journal of Power Sources, 2018, 388, 1-4.	7.8	12
101	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
102	First-principles study of the formation of glycine-producing radicals from common interstellar species. Molecular Astrophysics, 2018, 10, 11-19.	1.6	22
103	The binding structure and affinity of photodamaged duplex DNA with members of the photolyase/cryptochrome family: A computational study. Biophysics and Physicobiology, 2018, 15, 18-27.	1.0	7
104	Nonadiabatic one-electron transfer mechanism for the Oâ€“O bond formation in the oxygen-evolving complex of photosystem II. Chemical Physics Letters, 2018, 698, 138-146.	2.6	28
105	Molecular association model of PPARÎ± and its new specific and efficient ligand, pemafibrate: Structural basis for SPPARMÎ±. Biochemical and Biophysical Research Communications, 2018, 499, 239-245.	2.1	47
106	An assessment of optimal time scale of conformational resampling for parallel cascade selection molecular dynamics. Molecular Simulation, 2018, 44, 206-212.	2.0	6
107	The Formation of Hydrophobic Core Regulates the Protein Folding of Villin Elucidated with Parallel Cascade Selection Molecular Dynamics. Chemistry Letters, 2018, 47, 1300-1303.	1.3	0
108	Protein Residue Networks from Energetic and Geometric Data: Are They Identical?. Journal of Chemical Theory and Computation, 2018, 14, 6623-6631.	5.3	24

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109	A Theoretical Study on Redox Potential and pKa of [2Fe-2S] Cluster Model from Iron-Sulfur Proteins. Bulletin of the Chemical Society of Japan, 2018, 91, 1451-1456.	3.2	4
110	Reaction Pathway of Surface-Catalyzed Ammonia Decomposition and Nitrogen Incorporation in Epitaxial Growth of Gallium Nitride. Journal of Physical Chemistry C, 2018, 122, 24665-24671.	3.1	10
111	Synergetic Effects of Tripletâ€“Triplet Annihilation and Directional Triplet Exciton Migration in Organic Crystals for Photon Upconversion. Journal of Physical Chemistry Letters, 2018, 9, 6638-6643.	4.6	23
112	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
113	High-performance Na ion cathodes based on the ubiquitous and reversible O redox reaction. Journal of Materials Chemistry A, 2018, 6, 24120-24127.	10.3	5
114	Redox Potentialâ€Đependent Formation of an Unusual Hisâ€“Trp Bond in Bilirubin Oxidase. Chemistry - A European Journal, 2018, 24, 18052-18058.	3.3	14
115	Coulomb and CHâ€“Ï€Âinteractions in (6â€“4) photolyaseâ€“DNA complex dominate DNA binding and repair abilities. Nucleic Acids Research, 2018, 46, 6761-6772.	14.5	11
116	Concerted Mechanism of Water Insertion and O₂ Release during the S₄ to S₀ Transition of the Oxygen-Evolving Complex in PhotosystemÂII. Journal of Physical Chemistry B, 2018, 122, 6491-6502.	2.6	21
117	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
118	Novel Techniques for Observing Structural Dynamics of Photoresponsive Liquid Crystals. Journal of Visualized Experiments, 2018, , .	0.3	2
119	A Practical Approach for Searching Stable Molecular Structures by Introducing Repulsive Interactions among Walkers. Bulletin of the Chemical Society of Japan, 2018, 91, 1465-1473.	3.2	4
120	A computational scheme of pK_a values based on the three-dimensional reference interaction site model self-consistent field theory coupled with the linear fitting correction scheme. Physical Chemistry Chemical Physics, 2018, 20, 27272-27279.	2.8	11
121	Computational electrochemistry of a novel ferrocene derivative. Journal of Molecular Graphics and Modelling, 2018, 85, 84-90.	2.4	2
122	How Does Friction Coefficient Affect the Conformational Sampling Efficiency of Parallel Cascade Selection Molecular Dynamics?. Chemistry Letters, 2018, 47, 1119-1122.	1.3	1
123	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
124	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
125	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
126	Molecular Dynamics studies on the effects of Antifreezing Protein from Rhagium inquisitor (RiAFP) on Ice Growth. Journal of Computer Chemistry Japan, 2018, 17, 222-224.	0.1	0

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127	The Reaction Mechanisms of O₂ Formation in Photosynthesis. Seibutsu Butsuri, 2018, 58, 127-133.	0.1	0
128	Cooperatively Interlocked [2+1]â€Type Ï€â€Systemâ€“Anion Complexes. Chemistry - A European Journal, 2017, 23, 4160-4168.	3.3	17
129	Outstanding Reviewers for Physical Chemistry Chemical Physics in 2016. Physical Chemistry Chemical Physics, 2017, 19, 8140-8140.	2.8	0
130	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
131	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
132	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
133	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
134	Direct Observation of the Ultrafast Evolution of Open-Shell Biradical in Photochromic Radical Dimer. Journal of the American Chemical Society, 2017, 139, 6382-6389.	13.7	23
135	Structural dissimilarity sampling with dynamically self-guiding selection. Journal of Computational Chemistry, 2017, 38, 1921-1929.	3.3	11
136	Theoretical Analyses of Tripletâ€“Triplet Annihilation Process of 9,10-Diphenylanthracene in Solution. Chemistry Letters, 2017, 46, 873-875.	1.3	11
137	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
138	Theoretical study on relationship between spin structure and electron conductivity of one-dimensional tri-nickel(II) complex. Polyhedron, 2017, 136, 125-131.	2.2	8
139	Large-scale QM/MM calculations of the CaMn₄O₅ cluster in the S₃ state of the oxygen evolving complex of photosystem II. Comparison between water-inserted and no water-inserted structures. Faraday Discussions, 2017, 198, 83-106.	3.2	31
140	H-Aggregated Ï€-Systems Based on Disulfide-Linked Dimers of Dipyrrolyldiketone Boron Complexes. Journal of Organic Chemistry, 2017, 82, 11166-11172.	3.2	7
141	A theoretical study of the formation of glycine via hydantoin intermediate in outer space environment. Chemical Physics Letters, 2017, 687, 178-183.	2.6	22
142	Structural Monitoring of the Onset of Excited-State Aromaticity in a Liquid Crystal Phase. Journal of the American Chemical Society, 2017, 139, 15792-15800.	13.7	59
143	Classical cumulant dynamics for statistical chemical physics. Molecular Simulation, 2017, 43, 1260-1268.	2.0	0
144	Mechanistic Insight into Weak Baseâ€Catalyzed Generation of Carbon Monoxide from Phenyl Formate and Its Application to Catalytic Carbonylation at Room Temperature without Use of External Carbon Monoxide Gas. Advanced Synthesis and Catalysis, 2017, 359, 3592-3601.	4.3	19

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145	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
146	Temperatureâ€shuffled parallel cascade selection molecular dynamics accelerates the structural transitions of proteins. Journal of Computational Chemistry, 2017, 38, 2671-2674.	3.3	23
147	Assessment of Methodology and Chemical Group Dependences in the Calculation of the pK_a for Several Chemical Groups. Journal of Chemical Theory and Computation, 2017, 13, 4791-4803.	5.3	25
148	Phototransformative Supramolecular Assembly of Amphiphilic Diarylethenes Realized by a Combination of Photochromism and Lower Critical Solution Temperature Behavior. Chemistry - A European Journal, 2017, 23, 15059-15066.	3.3	15
149	Self-Avoiding Conformational Sampling Based on Histories of Past Conformational Searches. Journal of Chemical Information and Modeling, 2017, 57, 3070-3078.	5.4	7
150	Integrated Computational Studies on Mutational Effects of a Nylon-Degrading Enzyme. Progress in Theoretical Chemistry and Physics, 2017, , 317-330.	0.2	0
151	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
152	Refractive indices of organoâ€metallic and â€metalloid compounds: A longâ€range corrected DFT study. Journal of Computational Chemistry, 2016, 37, 2759-2769.	3.3	4
153	Mutations affecting the internal equilibrium of the reaction catalyzed by 6â€aminohexanoateâ€dimer hydrolase. FEBS Letters, 2016, 590, 3133-3143.	2.8	1
154	Ion-Pairing Crystal Polymorphs of Interlocked [2 + 1]-Type Receptorâ€“Anion Complexes. Journal of Organic Chemistry, 2016, 81, 8530-8536.	3.2	9
155	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
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