Noriaki Okimoto

List of Publications by Year
in descending order

49 papers	1,123 citations	471509 17 h-index	414414 32 g-index
53 all docs	53 docs citations	53 times ranked	1736 citing authors

#	Article	IF	Citations
1	High-Performance Drug Discovery: Computational Screening by Combining Docking and Molecular Dynamics Simulations. PLoS Computational Biology, 2009, 5, e1000528.	3.2	150
2	FGF9 monomerâ€“dimer equilibrium regulates extracellular matrix affinity and tissue diffusion. Nature Genetics, 2009, 41, 289-298.	21.4	104
3	Molecular Mechanisms of How Mercury Inhibits Water Permeation through Aquaporin-1: Understanding by Molecular Dynamics Simulation. Biophysical Journal, 2010, 98, 1512-1519.	0.5	86
4	Theoretical Studies of the ATP Hydrolysis Mechanism of Myosin. Biophysical Journal, 2001, 81, 2786-2794.	0.5	64
5	Folding Dynamics of 10-Residue Î²-Hairpin Peptide Chignolin. Chemistry - an Asian Journal, 2007, 2, 591-598.	3.3	54
6	Drug binding dynamics of the dimeric SARS-CoV-2 main protease, determined by molecular dynamics simulation. Scientific Reports, 2020, 10, 16986.	3.3	54
7	An Efficient Computational Method for Calculating Ligand Binding Affinities. PLoS ONE, 2012, 7, e42846.	2.5	46
8	Hydrolysis Mechanism of the Phenylalanineâ^'Proline Peptide Bond Specific to HIV-1 Protease:â€‰ Investigation by the ab Initio Molecular Orbital Method. Journal of the American Chemical Society, 1999, 121, 7349-7354.	13.7	43
9	Gordon Bell finalists II---A 55 TFLOPS simulation of amyloid-forming peptides from yeast prion Sup35 with the special-purpose computer system MDGRAPE-3. , 2006, , .		43
10	All-Atom Molecular Dynamics Simulations of Entire Virus Capsid Reveal the Role of Ion Distribution in Capsidâ€™s Stability. Journal of Physical Chemistry Letters, 2017, 8, 779-784.	4.6	42
11	Novel Mechanism of Interaction of p85 Subunit of Phosphatidylinositol 3-Kinase and ErbB3 Receptor-derived Phosphotyrosyl Peptides. Journal of Biological Chemistry, 2005, 280, 1321-1326.	3.4	40
12	Molecular Dynamics Study of HIV-1 Proteaseâ^'Substrate Complex:Â Roles of the Water Molecules at the Loop Structures of the Active Site. Journal of the American Chemical Society, 2000, 122, 5613-5622.	13.7	38
13	Tyr-317 Phosphorylation Increases Shc Structural Rigidity and Reduces Coupling of Domain Motions Remote from the Phosphorylation Site as Revealed by Molecular Dynamics Simulations. Journal of Biological Chemistry, 2004, 279, 4657-4662.	3.4	30
14	Free-Energy Landscapes of Protein Domain Movements upon Ligand Binding. Journal of Physical Chemistry B, 2011, 115, 7629-7636.	2.6	28
15	Assessment and acceleration of binding energy calculations for proteinâ€“ligand complexes by the fragment molecular orbital method. Journal of Computational Chemistry, 2015, 36, 2209-2218.	3.3	27
16	Computational Studies on Prion Proteins: Effect of Ala117â†'Val Mutation. Biophysical Journal, 2002, 82, 2746-2757.	0.5	23
17	Structure and dynamics of RNA polymerase II elongation complex. Biochemical and Biophysical Research Communications, 2006, 343, 90-98.	2.1	22
18	Petascale molecular dynamics simulation using the fast multipole method on K computer. Computer Physics Communications, 2014, 185, 2575-2585.	7.5	22

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19	Molecular Dynamics Study on Class A Î²-Lactamase: Hydrogen Bond Network among the Functional Groups of Penicillin G and Side Chains of the Conserved Residues in the Active Site. Journal of Physical Chemistry B, 2003, 107, 10274-10283.	2.6	18
20	Ligand Diffusion on Protein Surface Observed in Molecular Dynamics Simulation. Journal of Physical Chemistry Letters, 2012, 3, 3476-3479.	4.6	18
21	Single-Molecule Motions of MHC Class II Rely on Bound Peptides. Biophysical Journal, 2015, 108, 350-359.	0.5	16
22	Evaluation of proteinâ€“ligand affinity prediction using steered molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2017, 35, 3221-3231.	3.5	14
23	Use of the Multilayer Fragment Molecular Orbital Method to Predict the Rank Order of Proteinâ€“Ligand Binding Affinities: A Case Study Using Tankyrase 2 Inhibitors. ACS Omega, 2018, 3, 4475-4485.	3.5	14
24	Molecular Dynamics Study of Conformational Changes of Tankyrase 2 Binding Subsites upon Ligand Binding. ACS Omega, 2021, 6, 17609-17620.	3.5	14
25	Prediction of the Structure of Complexes Comprised of Proteins and Glycosaminoglycans Using Docking Simulation and Cluster Analysis. Journal of Chemical Theory and Computation, 2007, 3, 2347-2356.	5.3	13
26	A leukotriene C4 synthase inhibitor with the backbone of 5-(5-methylene-4-oxo-4,5-dihydrothiazol-2-ylamino) isophthalic acid. Journal of Biochemistry, 2013, 153, 421-429.	1.7	13
27	A new set of atomic radii for accurate estimation of solvation free energy by Poissonâ€“Boltzmann solvent model. Journal of Computational Chemistry, 2014, 35, 2132-2139.	3.3	13
28	Molecular Dynamics Simulations of Prion Proteins-Effect of Ala117 .RAR.Val mutation-. Chem-Bio Informatics Journal, 2003, 3, 1-11.	0.3	12
29	Cooperative Motions of Protein and Hydration Water Molecules:Â Molecular Dynamics Study of Scytalone Dehydratase. Journal of the American Chemical Society, 2004, 126, 13132-13139.	13.7	12
30	Acid-catalyzed deprotection mechanism oftert-butyloxycarbonyloxy polymers in chemically amplified resists. Journal of Polymer Science Part A, 1998, 36, 1035-1042.	2.3	10
31	Comparison of binding affinity evaluations for FKBP ligands with state-of-the-art computational methods: FMO, QM/MM, MM-PB/SA and MP-CAFEE approaches. Chem-Bio Informatics Journal, 2010, 10, 32-45.	0.3	9
32	A pre-metazoan origin of the CRK gene family and co-opted signaling network. Scientific Reports, 2016, 6, 34349.	3.3	7
33	Refolding molecular dynamics simulations of small- and middle-sized proteins in an explicit solvent. Molecular Simulation, 2002, 28, 337-357.	2.0	5
34	Behavior of water molecules in ATPase pocket of myosin. Computational and Theoretical Chemistry, 2006, 758, 97-105.	1.5	4
35	Theoretical insights into the DNA repair function of Arabidopsis thaliana cryptochrome-DASH. Biophysics and Physicobiology, 2020, 17, 113-124.	1.0	4
36	Improvement of Sampling Efficiency through Combined use of Molecular Dynamics Simulations with Implicit and Explicit Solvent Models. Biophysical Journal, 2013, 104, 170a-171a.	0.5	2

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37	A novel bovine leukemia virus peptide vaccine targeting susceptible cattle-Production by 3-D modelling and nanotechnology. Retrovirology, 2015, 12, .	2.0	2
38	Gag Protein Hydrolysis Mechanism by HIV-1 Protease. Investigation by Semiempirical Molecular Orbital Method.. Nippon Kagaku Kaishi / Chemical Society of Japan - Chemistry and Industrial Chemistry Journal, 1997, 1997, 260-266.	0.1	1
39	The Importance of OH groups Containing in Solid Films for High Sensitivity of Chemically Amplified Resists.. Journal of Photopolymer Science and Technology = [Fotoporima Konwakai Shi], 2000, 13, 503-506.	0.3	1
40	Quantum chemical analysis of reaction indices and reaction path for drug molecules. Journal of Physics: Conference Series, 2019, 1290, 012021.	0.4	1
41	Constant pH molecular dynamics of porcine circovirus 2 capsid protein reveals a mechanism for capsid assembly. Physical Chemistry Chemical Physics, 2021, 23, 24617-24626.	2.8	1
42	Molecular dynamics investigation of the double stranded oligonucleotide d(AT)6d(AT)6. Nucleic Acids Symposium Series, 2002, 2, 175-176.	0.3	0
43	2P061 Investigation of Domain Motions in Proteins by Molecular Dynamics Simulations(Proteins-structure and structure-function relationship,Poster Presentations). Seibutsu Butsuri, 2007, 47, S128.	0.1	0
44	3P089 Computational Analysis on Selectivity of Protein Kinase Inhibitors(Protein: Function,The 48th) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.1	0
45	Molecular Mechanisms How Mercury Inhibits Water Permeation of Aquaporin-1: Understanding by Molecular Dynamics Simulation. Biophysical Journal, 2010, 98, 568a.	0.5	0
46	Exploration of Free-Energy Profiles With Conformational Changes of Proteins. Biophysical Journal, 2010, 98, 26a.	0.5	0
47	1PT188 Improvement of sampling efficiency through combined use of molecular dynamics simulations with implicit and explicit solvent models(The 50th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2012, 52, S101.	0.1	0
48	[Special Issue for Honor Award dedicating to Prof Kimito Funatsu]Fast Evaluation of Potential Synthesis Routes Using Transition State Database(TSDB). Journal of Computer Aided Chemistry, 2019, 20, 50-55.	0.3	0
49	Theoretical Analyses for DNA Repair Function of Cryptochrome-DASH. Seibutsu Butsuri, 2022, 62, 116-118.	0.1	0