Kota Kasahara

List of Publications by Year in Descending Order

42 papers	486 citations	12 h-index	21 g-index
45 ext. papers	604 ext. citations	4.3 avg, IF	3.97 L-index

#	Paper	IF	Citations
42	Extended ensemble simulations of a SARS-CoV-2 nsp1-5′-UTR complex.. *PLoS Computational Biology* , **2022**, 18, e1009804	5	1
41	Information quantity for secondary structure propensities of protein subsequences in the Protein Data Bank.. *Biophysics and Physicobiology*, **2022**, 19, 1-12	1.4	
40	Difference of binding modes among three ligands to a receptor mSin3B corresponding to their inhibitory activities. *Scientific Reports*, **2021**, 11, 6178	4.9	0
39	All-Atom Molecular Dynamics Elucidating Molecular Mechanisms of Single-Transmembrane Model Peptide Dimerization in a Lipid Bilayer. *ACS Omega*, **2021**, 6, 11458-11465	3.9	0
38	New Protocol for Predicting the Ligand-Binding Site and Mode Based on the 3D-RISM/KH Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 2864-2876	6.4	9
37	GA-guided mD-VcMD: A genetic-algorithm-guided method for multi-dimensional virtual-system coupled molecular dynamics. *Biophysics and Physicobiology*, **2020**, 17, 161-176	1.4	4
36	myPresto/omegagene 2020: a molecular dynamics simulation engine for virtual-system coupled sampling. *Biophysics and Physicobiology*, **2020**, 17, 140-146	1.4	5
35	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	6.1	3
34	Effects of ion–water Lennard-Jones potentials on the hydration dynamics around a monovalent atomic ion in molecular dynamics simulations. *Molecular Simulation*, **2020**, 46, 83-91	2	1
33	Gene Cascade Finder: A tool for identification of gene cascades and its application in Caenorhabditis elegans. *PLoS ONE*, **2019**, 14, e0215187	3.7	3
32	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	1.9	7
31	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	6.4	13
30	Multidimensional virtual-system coupled canonical molecular dynamics to compute free-energy landscapes of peptide multimer assembly. *Journal of Computational Chemistry*, **2019**, 40, 2453-2463	3.5	7
29	Studies on Molecular Dynamics of Intrinsically Disordered Proteins and Their Fuzzy Complexes: A Mini-Review. *Computational and Structural Biotechnology Journal*, **2019**, 17, 712-720	6.8	22
28	Molecular dynamics coupled with a virtual system for effective conformational sampling. *Journal of Computational Chemistry*, **2018**, 39, 1291-1299	3.5	5
27	Enhanced Sampling of Molecular Dynamics Simulations of a Polyalanine Octapeptide: Effects of the Periodic Boundary Conditions on Peptide Conformation. *Journal of Physical Chemistry B*, **2018**, 122, 2495-2503	3.4	12
26	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	20.1	22

25	Influence of various parameters in the replica-exchange molecular dynamics method: Number of replicas, replica-exchange frequency, and thermostat coupling time constant. *Biophysics and Physicobiology*, **2018**, 15, 165-172	1.4	4
24	Unfolding of α-helical 20-residue poly-glutamic acid analyzed by multiple runs of canonical molecular dynamics simulations. *PeerJ*, **2018**, 6, e4769	3.1	3
23	Characteristics of interactions at protein segments without non-local intramolecular contacts in the Protein Data Bank. *PLoS ONE*, **2018**, 13, e0205052	3.7	1
22	Enhancement of canonical sampling by virtual-state transitions. *Journal of Chemical Physics*, **2017**, 146, 044104	3.9	12
21	Multi-dimensional virtual system introduced to enhance canonical sampling. *Journal of Chemical Physics*, **2017**, 147, 134102	3.9	7
20	Molecular mechanisms of cooperative binding of transcription factors Runx1-CBFβ-Ets1 on the TCRα gene enhancer. *PLoS ONE*, **2017**, 12, e0172654	3.7	8
19	An FPGA Accelerator for Molecular Dynamics Simulation Using OpenCL. *International Journal of Networked and Distributed Computing*, **2017**, 5, 52	1.3	3
18	myPresto/omegagene: a GPU-accelerated molecular dynamics simulator tailored for enhanced conformational sampling methods with a non-Ewald electrostatic scheme. *Biophysics and Physicobiology*, **2016**, 13, 209-216	1.4	16
17	Ion Concentration- and Voltage-Dependent Push and Pull Mechanisms of Potassium Channel Ion Conduction. *PLoS ONE*, **2016**, 11, e0150716	3.7	5
16	IBiSA_Tools: A Computational Toolkit for Ion-Binding State Analysis in Molecular Dynamics Trajectories of Ion Channels. *PLoS ONE*, **2016**, 11, e0167524	3.7	1
15	Landscape of protein-small ligand binding modes. *Protein Science*, **2016**, 25, 1659-71	6.3	3
14	mDCC_tools: characterizing multi-modal atomic motions in molecular dynamics trajectories. *Bioinformatics*, **2016**, 32, 2531-3	7.2	2
13	Architecture of an FPGA accelerator for molecular dynamics simulation using OpenCL **2016**,		5
12	Virtual-system-coupled adaptive umbrella sampling to compute free-energy landscape for flexible molecular docking. *Journal of Computational Chemistry*, **2015**, 36, 1489-501	3.5	26
11	GIANT: pattern analysis of molecular interactions in 3D structures of protein-small ligand complexes. *BMC Bioinformatics*, **2014**, 15, 12	3.6	13
10	Specific non-local interactions are not necessary for recovering native protein dynamics. *PLoS ONE*, **2014**, 9, e91347	3.7	2
9	A novel approach of dynamic cross correlation analysis on molecular dynamics simulations and its application to Ets1 dimer-DNA complex. *PLoS ONE*, **2014**, 9, e112419	3.7	65
8	Comprehensive classification and diversity assessment of atomic contacts in protein-small ligand interactions. *Journal of Chemical Information and Modeling*, **2013**, 53, 241-8	6.1	10

7	Ion concentration-dependent ion conduction mechanism of a voltage-sensitive potassium channel. *PLoS ONE*, **2013**, 8, e56342	3.7	12
6	ATTED-II updates: condition-specific gene coexpression to extend coexpression analyses and applications to a broad range of flowering plants. *Plant and Cell Physiology*, **2011**, 52, 213-9	4.9	133
5	Ligand-binding site prediction of proteins based on known fragment-fragment interactions. *Bioinformatics*, **2010**, 26, 1493-9	7.2	14
4	Tight-Binding Quantum Chemical Molecular Dynamics Study on First Proton Transfer Process of ORR Catalyzed by Cobalt-Porphyrin Complex. *Electrochemical and Solid-State Letters*, **2006**, 9, A490		19
3	Molecular interaction mechanism of a 14-3-3 protein with a phosphorylated peptide elucidated by enhanced conformational sampling		2
2	Effects of number of parallel runs and frequency of bias-strength replacement in generalized ensemble molecular dynamics simulations1, e4		2
1	Modeling the SARS-CoV-2 nsp1□□UTR complex via extended ensemble simulations		2