Yoshitake Sakae

List of Publications by Year
in descending order

24	446	1040056 9	794594 19
papers	citations	h-index	g-index

25	25	25	760
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Combination of genetic algorithm and generalised-ensemble algorithms for biomolecular simulations. Frontiers of Nanoscience, 2022, , 93-109.	0.6	0
2	Absolute Protein Binding Free Energy Simulations for Ligands with Multiple Poses, a Thermodynamic Path That Avoids Exhaustive Enumeration of the Poses. Journal of Computational Chemistry, 2020, 41, 56-68.	3.3	16
3	N+-C-HÂ·Â·Â·O Hydrogen bonds in protein-ligand complexes. Scientific Reports, 2019, 9, 767.	3.3	81
4	Structural Analysis of a Trimer of Î²2-Microgloblin Fragment by Molecular Dynamics Simulations. Biophysical Journal, 2019, 116, 781-790.	0.5	3
5	Enhanced sampling method in molecular simulations using genetic algorithm for biomolecular systems. Journal of Computational Chemistry, 2019, 40, 475-481.	3.3	3
6	Computational analysis for selectivity of histone deacetylase inhibitor by replica-exchange umbrella sampling molecular dynamics simulations. Journal of Chemical Physics, 2018, 148, 125102.	3.0	7
7	Structureâ€“function insights into direct lipid transfer between membranes by Mmm1â€“Mdm12 of ERMES. Journal of Cell Biology, 2018, 217, 959-974.	5.2	116
8	Conformational effects of N-glycan core fucosylation of immunoglobulin G Fc region on its interaction with FcÎ³ receptor IIIa. Scientific Reports, 2017, 7, 13780.	3.3	57
9	Two major stable structures of amyloid-forming peptides: amorphous aggregates and amyloid fibrils. Molecular Simulation, 2017, 43, 1370-1376.	2.0	5
10	<Review> A Mini-review on Chemoinformatics Approaches for Drug Discovery. Journal of Computer Aided Chemistry, 2015, 16, 15-29.	0.3	6
11	Molecular Dynamics Simulations to Clarify the Concentration Dependency of Protein Aggregation. , 2015, , .		1
12	Conformational search simulations of Trp-cage using genetic crossover. Molecular Simulation, 2015, 41, 1045-1049.	2.0	3
13	A Conformational Search Method for Protein Systems Using Genetic Crossover and Metropolis Criterion. Journal of Physics: Conference Series, 2014, 487, 012003.	0.4	8
14	Exploration of Conformational Spaces of Highâ€Mannoseâ€Type Oligosaccharides by an NMRâ€Validated Simulation. Angewandte Chemie - International Edition, 2014, 53, 10941-10944.	13.8	60
15	Improvement of the backbone-torsion-energy term in the force field for protein systems by the double Fourier series expansion. Molecular Simulation, 2013, 39, 85-93.	2.0	2
16	3G1346 Protein Structure Predictions by Simulated Annealing Molecular Dynamics Using Genetic Crossover(3G Protein: Structure 4,The 49th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2011, 51, S131.	0.1	0
17	Protein structure predictions by parallel simulated annealing molecular dynamics using genetic crossover. Journal of Computational Chemistry, 2011, 32, 1353-1360.	3.3	16
18	3P018 A Simulated Annealing Molecular Dynamics Using Genetic Crossover with Knot Theory(Protein:) Tj ETQq0 0 0 rgBT /Overlock 10 T S148.	0.1	0

#	Article	IF	Citations
19	Optimisation of OPLSâ€“UA force-field parameters for protein systems using protein data bank. Molecular Simulation, 2010, 36, 1148-1156.	2.0	10
20	Controlling the secondary-structure-forming tendencies of proteins by a backbone torsion-energy term. Molecular Simulation, 2010, 36, 138-158.	2.0	9
21	Determination method of the balance of the secondary-structure-forming tendencies of force fields. Molecular Simulation, 2010, 36, 159-165.	2.0	4
22	Folding simulations of three proteins having all Î±-helix, all Î²-strand and Î±/Î²-structures. Molecular Simulation, 2010, 36, 302-310.	2.0	8
23	3P-056 A simulated annealing molecular dynamics simulation with a genetic crossover for protein systems(Protein:Property,The 47th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2009, 49, S160.	0.1	0
24	Optimization of protein force-field parameters with the Protein Data Bank. Chemical Physics Letters, 2003, 382, 626-636.	2.6	31