Koji Ogata

List of Publications by Year in descending order

45 papers	1,979 citations	361413 20 h-index	315739 38 g-index
45 all docs	45 docs citations	45 times ranked	3333 citing authors

#	Article	IF	Citations
1	Investigation of Cooperative Modes for Collective Molecules Using Grid-Based Principal Component Analysis. Journal of Physical Chemistry B, 2021, 125, 1072-1084.	2.6	1
2	Identification of novel bacterial urease inhibitors through molecular shape and structure based virtual screening approaches. RSC Advances, 2020, 10, 16061-16070.	3.6	26
3	Investigation of a Pathway for Water Delivery in Photosystem II Protein by Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2019, 123, 6444-6452.	2.6	10
4	Effect of Atomic Charges on Octanolâ€“Water Partition Coefficient Using Alchemical Free Energy Calculation. Molecules, 2018, 23, 425.	3.8	16
5	A study on an unusual SN2 mechanism in the methylation of benzyne through nickel-complexation. Physical Chemistry Chemical Physics, 2017, 19, 26926-26933.	2.8	4
6	Unusual Ionic Bond and Solubility Mechanism of Na_nPQQ (n = 0â€“4) Crystals. Crystal Growth and Design, 2017, 17, 4118-4123.	3.0	5
7	Boltzmann Sampling by Degenerate Optical Parametric Oscillator Network for Structure-Based Virtual Screening. Entropy, 2016, 18, 365.	2.2	31
8	Diastereomeric resolution directed towards chirality determination focussing on gas-phase energetics of coordinated sodium dissociation. Scientific Reports, 2016, 6, 24005.	3.3	7
9	Structural changes in the S3 state of the oxygen evolving complex in photosystem II. Chemical Physics Letters, 2016, 651, 243-250.	2.6	17
10	A model study of hydrothermal reactions of trigonal dipyramidal Zn5 cluster with two water molecules. Computational and Theoretical Chemistry, 2015, 1070, 126-131.	2.5	3
11	Theoretical Study on Carbonâ€“Carbon Short Contact of â¼2.3 Ã…: Intermediate State between Nonbonding and Ïƒ-Covalent Bonding. Journal of Physical Chemistry A, 2015, 119, 781-785.	2.5	1
12	Quality Assessment of Predicted Protein Models Using Energies Calculated by the Fragment Molecular Orbital Method. Molecular Informatics, 2015, 34, 97-104.	2.5	13
13	Improvement of Parameters of the AMBER Potential Force Field for Phospholipids for Description of Thermal Phase Transitions. Journal of Physical Chemistry B, 2015, 119, 9726-9739.	2.6	20
14	Activation of CO₂by ionic liquid EMIMâ€“BF₄in the electrochemical system: a theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 23521-23531.	2.8	101
15	A Basic Quantum Chemical Review on the Activation of CO₂. ACS Symposium Series, 2015, , 123-134.	0.5	7
16	Theoretical Study on the Role of Ca²⁺ at the S₂ State in Photosystem II. Journal of Physical Chemistry B, 2014, 118, 14215-14222.	2.6	30
17	Understanding Thermal Phases in Atomic Detail by All-Atom Molecular-Dynamics Simulation of a Phospholipid Bilayer. Journal of Physical Chemistry B, 2014, 118, 14353-14365.	2.6	10
18	New insights into highly efficient reduction of CO₂to formic acid by using zinc under mild hydrothermal conditions: a joint experimental and theoretical study. Physical Chemistry Chemical Physics, 2014, 16, 19836.	2.8	23

#	Article	IF	Citations
19	Binding Free-Energy Calculation Is a Powerful Tool for Drug Optimization: Calculation and Measurement of Binding Free Energy for 7-Azaindole Derivatives to Glycogen Synthase Kinase-3Î². Journal of Chemical Information and Modeling, 2014, 54, 1653-1660.	5.4	24
20	All-Atom Molecular Dynamics Simulation of Photosystem II Embedded in Thylakoid Membrane. Journal of the American Chemical Society, 2013, 135, 15670-15673.	13.7	82
21	A study of QM/Langevin-MD simulation for oxygen-evolving center of photosystem II. , 2013, , .		0
22	Theoretical study on OH[sup â^'] site and electronic spin state of oxygen-evolving complex in photosystem II at the dark S[sub 1] state. , 2013, , .		0
23	Theoretical investigation on single-molecule chiroptical spectroscopy. , 2013, , .		0
24	Unrestricted Hartree-Fock based on the fragment molecular orbital method: Energy and its analytic gradient. Journal of Chemical Physics, 2012, 137, 044110.	3.0	35
25	MD Simulation Study of Ras/Raf Dissociation and the Resonating Structure of Deactivated Ras. Bulletin of the Chemical Society of Japan, 2012, 85, 1318-1328.	3.2	3
26	Photochromism of 1,2-Bis(2-thienyl)perfluorocyclopentene Derivatives: Substituent Effect on the Reactive Carbon Atoms. Journal of Physical Chemistry A, 2012, 116, 10973-10979.	2.5	22
27	Direct binding targets of the stringent response alarmone (p)ppGpp. Molecular Microbiology, 2012, 85, 1029-1043.	2.5	153
28	Activators of Cylindrical Proteases as Antimicrobials: Identification and Development of Small Molecule Activators of ClpP Protease. Chemistry and Biology, 2011, 18, 1167-1178.	6.0	86
29	Mutations in chaperonin-like BBS genes are a major contributor to disease development in a multiethnic Bardet-Biedl syndrome patient population. Journal of Medical Genetics, 2010, 47, 453-463.	3.2	84
30	Lead Generation and Optimization Based on Protein-Ligand Complementarity. Molecules, 2010, 15, 4382-4400.	3.8	9
31	An electrostatic switch displaces phosphatidylinositol phosphate kinases from the membrane during phagocytosis. Journal of General Physiology, 2010, 135, i1-i1.	1.9	0
32	An electrostatic switch displaces phosphatidylinositol phosphate kinases from the membrane during phagocytosis. Journal of Cell Biology, 2009, 187, 701-714.	5.2	86
33	Mincle is an ITAM-coupled activating receptor that senses damaged cells. Nature Immunology, 2008, 9, 1179-1188.	14.5	627
34	A Quantitative Approach to the Estimation of Chemical Space from a Given Geometry by the Combination of Atomic Species. QSAR and Combinatorial Science, 2007, 26, 596-607.	1.4	21
35	CRYBA4, a Novel Human Cataract Gene, Is Also Involved in Microphthalmia. American Journal of Human Genetics, 2006, 79, 702-709.	6.2	87
36	Mechanistic basis of preâ€“T cell receptorâ€“mediated autonomous signaling critical for thymocyte development. Nature Immunology, 2006, 7, 67-75.	14.5	133

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37	A Monte Carlo Sampling Method of Amino Acid Sequences Adaptable to Given Main-Chain Atoms in the Proteins. Journal of Biochemistry, 2006, 140, 543-552.	1.7	0
38	Automatic Sequence Design of Major Histocompatibility Complex Class I Binding Peptides Impairing CD8+ T Cell Recognition. Journal of Biological Chemistry, 2003, 278, 1281-1290.	3.4	32
39	Conserved water molecules in MHC class-I molecules and their putative structural and functional roles. Protein Engineering, Design and Selection, 2002, 15, 697-705.	2.1	53
40	Modeling the three-dimensional structure of H+-ATPase ofNeurospora crassa. FEBS Journal, 2002, 269, 5246-5258.	0.2	6
41	An automatic homology modeling method consisting of database searches and simulated annealing. Journal of Molecular Graphics and Modelling, 2000, 18, 258-272.	2.4	83
42	Multiple alignment for amino acid sequences by dynamic programming. Electronics and Communications in Japan, Part III: Fundamental Electronic Science (English Translation of Denshi) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.1	3
43	The role played by environmental residues on sidechain torsional angles within homologous families of proteins: A new method of sidechain modeling. Proteins: Structure, Function and Bioinformatics, 1998, 31, 355-369.	2.6	15
44	Amino acid similarity matrix for homology modeling derived from structural alignment and optimized by the Monte Carlo method. Journal of Molecular Graphics and Modelling, 1998, 16, 178-189.	2.4	13
45	The role played by environmental residues on sidechain torsional angles within homologous families of proteins: A new method of sidechain modeling. Proteins: Structure, Function and Bioinformatics, 1998, 31, 355-369.	2.6	0