

Takeshi Yamazaki

List of Publications by Year in descending order

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43
papers

1,169
citations

331259

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docs citations

44
times ranked

1253
citing authors

#	ARTICLE	IF	CITATIONS
1	Size Selective Corona Interactions from Self-Assembled Rosette and Single-Walled Carbon Nanotubes. <i>Small</i> , 2022, 18, e2104951.	5.2	2
2	Anti-Tumor Effects of Ginsenoside 20(S)-Protopanaxadiol and 1,25-Dihydroxyvitamin D3 Combination in Castration Resistant Prostate Cancer. <i>Medicines (Basel, Switzerland)</i> , 2021, 8, 28.	0.7	3
3	Scaling up electronic structure calculations on quantum computers: The frozen natural orbital based method of increments. <i>Journal of Chemical Physics</i> , 2021, 155, 034110.	1.2	15
4	Optimizing electronic structure simulations on a trapped-ion quantum computer using problem decomposition. <i>Communications Physics</i> , 2021, 4, .	2.0	23
5	Nuclear magnetic shielding of molecule in solution based on reference interaction site model self-consistent field with spatial electron density distribution. <i>Journal of Chemical Physics</i> , 2020, 152, 194102.	1.2	5
6	A molecular reconstruction approach to site-based 3D-RISM and comparison to GIST hydration thermodynamic maps in an enzyme active site. <i>PLoS ONE</i> , 2019, 14, e0219473.	1.1	22
7	Ivermectin inhibits HSP27 and potentiates efficacy of oncogene targeting in tumor models. <i>Journal of Clinical Investigation</i> , 2019, 130, 699-714.	3.9	36
8	Toxic Colors: The Use of Deep Learning for Predicting Toxicity of Compounds Merely from Their Graphic Images. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1533-1543.	2.5	101
9	Benzothiophenone Derivatives Targeting Mutant Forms of Estrogen Receptor- α in Hormone-Resistant Breast Cancers. <i>International Journal of Molecular Sciences</i> , 2018, 19, 579.	1.8	9
10	20(S)-protopanaxadiol regio-selectively targets androgen receptor: anticancer effects in castration-resistant prostate tumors. <i>Oncotarget</i> , 2018, 9, 20965-20978.	0.8	12
11	Discovery and characterization of small molecules targeting the DNA-binding ETS domain of ERG in prostate cancer. <i>Oncotarget</i> , 2017, 8, 42438-42454.	0.8	37
12	Encapsulation of ferrocene by self-assembled rosette nanotubes: An investigation using statistical mechanical theory of molecular liquids. <i>Journal of Molecular Liquids</i> , 2016, 217, 70-74.	2.3	3
13	High Field Solid-State NMR Spectroscopy Investigation of ¹⁵ N-Labeled Rosette Nanotubes: Hydrogen Bond Network and Channel-Bound Water. <i>Journal of the American Chemical Society</i> , 2016, 138, 6115-6118.	6.6	22
14	Small molecule hydration energy and entropy from 3D-RISM. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 344002.	0.7	39
15	Targeting Binding Function-3 of the Androgen Receptor Blocks Its Co-Chaperone Interactions, Nuclear Translocation, and Activation. <i>Molecular Cancer Therapeutics</i> , 2016, 15, 2936-2945.	1.9	24
16	Cheminformatics Modeling of Adverse Drug Responses by Clinically Relevant Mutants of Human Androgen Receptor. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 2507-2516.	2.5	16
17	Fluorescent Rosette Nanotubes from the C-analogue of the Guanine-Cytosine (G \hat{C}) Motif. <i>Materials Research Society Symposia Proceedings</i> , 2015, 1796, 1-6.	0.1	1
18	Functionalized Rosette Nanotubes as Novel Electron Donor Materials for Solution-Processed Organic Photovoltaics. <i>Materials Research Society Symposia Proceedings</i> , 2015, 1737, 1.	0.1	4

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19	Chiomers: conformation-driven mirror-image supramolecular chirality isomerism identified in a new class of helical rosette nanotubes. <i>Nanoscale</i> , 2014, 6, 9421-9427.	2.8	23
20	Synthesis of N-substituted Pyrido[4,3- <i>d</i>]pyrimidines for the Large-Scale Production of Self-Assembled Rosettes and Nanotubes. <i>Journal of Organic Chemistry</i> , 2013, 78, 11421-11426.	1.7	14
21	Imaging Carbon Nanotube Interaction with Nucleobases in Water Using the Statistical Mechanical Theory of Molecular Liquids. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15087-15092.	1.5	13
22	Covalent Capture of Self-Assembled Rosette Nanotubes. <i>Macromolecules</i> , 2012, 45, 7157-7162.	2.2	9
23	Synthesis of rhenium chelated MAG3 functionalized rosette nanotubes. <i>Tetrahedron Letters</i> , 2012, 53, 1645-1651.	0.7	8
24	Spatial Decomposition of Solvation Free Energy Based on the 3D Integral Equation Theory of Molecular Liquid: Application to Mini-proteins. <i>Journal of Physical Chemistry B</i> , 2011, 115, 310-318.	1.2	24
25	Self-Assembly of a Water-Soluble Tricyclic Heterocycle into J-Type Rosette Nanotubes. <i>Materials Research Society Symposia Proceedings</i> , 2011, 1312, 1.	0.1	0
26	Structural Water Drives Self-Assembly of Organic Rosette Nanotubes and Holds Host Atoms in the Channel. <i>ChemPhysChem</i> , 2010, 11, 361-367.	1.0	43
27	Ion Solvation in a Water-Urea Mixture. <i>Journal of Physical Chemistry B</i> , 2010, 114, 613-619.	1.2	28
28	One-Pot Nucleation, Growth, Morphogenesis, and Passivation of 1.4 nm Au Nanoparticles on Self-Assembled Rosette Nanotubes. <i>Journal of the American Chemical Society</i> , 2010, 132, 32-33.	6.6	47
29	Rosette nanotubes with 1.4 nm inner diameter from a tricyclic variant of the Lehn-Macaluso base. <i>Chemical Communications</i> , 2010, 46, 6527.	2.2	29
30	Water-Soluble J-Type Rosette Nanotubes with Giant Molar Ellipticity. <i>Journal of the American Chemical Society</i> , 2010, 132, 15136-15139.	6.6	61
31	Supramolecular Synthesis of Solid-State Tapes Through Molecular Facial Self-Recognition. <i>Helvetica Chimica Acta</i> , 2009, 92, 1963-1972.	1.0	1
32	Spatial Decomposition Analysis of the Thermodynamics of Cyclodextrin Complexation. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1723-1730.	2.3	24
33	Essential Role of Hydration in Aggregation of Misfolded Prion Proteins: Quantification by Molecular Theory of Solvation. <i>Journal of Toxicology and Environmental Health - Part A: Current Issues</i> , 2009, 72, 1060-1068.	1.1	0
34	Hydration Effects on the HET-s Prion and Amyloid- β Fibrillous Aggregates, Studied with Three-Dimensional Molecular Theory of Solvation. <i>Biophysical Journal</i> , 2008, 95, 4540-4548.	0.2	45
35	Hierarchical Self-Assembly of Organic Prolate Nanospheroids from Hydrophobic Rosette Nanotubes. <i>Langmuir</i> , 2008, 24, 4447-4450.	1.6	34
36	Molecular Basis for Water-Promoted Supramolecular Chirality Inversion in Helical Rosette Nanotubes. <i>Journal of the American Chemical Society</i> , 2007, 129, 5735-5743.	6.6	184

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37	Theoretical Study of the Cosolvent Effect on the Partial Molar Volume Change of Staphylococcal Nuclease Associated with Pressure Denaturation. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1206-1212.	1.2	24
38	Helical Rosette Nanotubes with Tunable Stability and Hierarchy. <i>Journal of the American Chemical Society</i> , 2005, 127, 8307-8309.	6.6	134
39	A quantum solute-solvent interaction using spectral representation technique applied to the electronic structure theory in solution. <i>Journal of Chemical Physics</i> , 2003, 119, 6663-6670.	1.2	11
40	Solvent effect on the nuclear magnetic shielding:ab initio study by the combined reference interaction site model and electronic structure theories. <i>Journal of Chemical Physics</i> , 2001, 115, 8949-8957.	1.2	17
41	NMR chemical shifts in solution: a RISM-SCF approach. <i>Chemical Physics Letters</i> , 2000, 325, 668-674.	1.2	17
42	A method for calculating electric dipole transition moments using small configuration interaction spaces based on the concept of interaction frontier orbitals. <i>Chemical Physics Letters</i> , 1998, 295, 431-438.	1.2	3
43	PSYCHOLOGICAL ASPECTS OF X-RAY SURFACE DIAGNOSIS OF THE DIGESTIVE TRACT RELATED TO VISUAL PERCEPTION. <i>Japanese Journal of Radiological Technology</i> , 1977, 33, 483-489.	0.0	0