

Takeshi Yamazaki

List of Publications by Year in descending order

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Version: 2024-02-01

43
papers

1,169
citations

331259

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377514

34
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44
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docs citations

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times ranked

1253
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|---|-----|-----------|
| 1 | 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 |
| 2 | Helical Rosette Nanotubes with Tunable Stability and Hierarchy. <i>Journal of the American Chemical Society</i> , 2005, 127, 8307-8309. | 6.6 | 134 |
| 3 | 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 |
| 4 | 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 |
| 5 | 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 |
| 6 | Hydration Effects on the HET-s Prion and Amyloid- β^2 Fibrillous Aggregates, Studied with Three-Dimensional Molecular Theory of Solvation. <i>Biophysical Journal</i> , 2008, 95, 4540-4548. | 0.2 | 45 |
| 7 | 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 |
| 8 | Small molecule hydration energy and entropy from 3D-RISM. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 344002. | 0.7 | 39 |
| 9 | 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 |
| 10 | 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 |
| 11 | Hierarchical Self-Assembly of Organic Prolate Nanospheroids from Hydrophobic Rosette Nanotubes. <i>Langmuir</i> , 2008, 24, 4447-4450. | 1.6 | 34 |
| 12 | Rosette nanotubes with 1.4 nm inner diameter from a tricyclic variant of the Lehn's Mascal G β S β C base. <i>Chemical Communications</i> , 2010, 46, 6527. | 2.2 | 29 |
| 13 | Ion Solvation in a Water-Urea Mixture. <i>Journal of Physical Chemistry B</i> , 2010, 114, 613-619. | 1.2 | 28 |
| 14 | 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 |
| 15 | Spatial Decomposition Analysis of the Thermodynamics of Cyclodextrin Complexation. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1723-1730. | 2.3 | 24 |
| 16 | Spatial Decomposition of Solvation Free Energy Based on the 3D Integral Equation Theory of Molecular Liquid: Application to Miniproteins. <i>Journal of Physical Chemistry B</i> , 2011, 115, 310-318. | 1.2 | 24 |
| 17 | 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 |
| 18 | Chromers: 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 |

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|----|--|-----|-----------|
| 19 | Optimizing electronic structure simulations on a trapped-ion quantum computer using problem decomposition. <i>Communications Physics</i> , 2021, 4, . | 2.0 | 23 |
| 20 | 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 |
| 21 | 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 |
| 22 | NMR chemical shifts in solution: a RISM-SCF approach. <i>Chemical Physics Letters</i> , 2000, 325, 668-674. | 1.2 | 17 |
| 23 | Solvent effect on the nuclear magnetic shielding: a 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 |
| 24 | 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 |
| 25 | 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 |
| 26 | 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 |
| 27 | 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 |
| 28 | 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 |
| 29 | 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 |
| 30 | Covalent Capture of Self-Assembled Rosette Nanotubes. <i>Macromolecules</i> , 2012, 45, 7157-7162. | 2.2 | 9 |
| 31 | 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 |
| 32 | Synthesis of rhenium chelated MAG3 functionalized rosette nanotubes. <i>Tetrahedron Letters</i> , 2012, 53, 1645-1651. | 0.7 | 8 |
| 33 | 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 |
| 34 | 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 |
| 35 | 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 |
| 36 | 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 |

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|----|--|-----|-----------|
| 37 | 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 |
| 38 | Size Selective Corona Interactions from Self-Assembled Rosette and Single-Walled Carbon Nanotubes. <i>Small</i> , 2022, 18, e2104951. | 5.2 | 2 |
| 39 | Supramolecular Synthesis of Solid-State Tapes Through Molecular Facial Self-Recognition. <i>Helvetica Chimica Acta</i> , 2009, 92, 1963-1972. | 1.0 | 1 |
| 40 | Fluorescent Rosette Nanotubes from the C-analogue of the Guanine-Cytosine (G ⁺ SC) Motif. <i>Materials Research Society Symposia Proceedings</i> , 2015, 1796, 1-6. | 0.1 | 1 |
| 41 | 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 |
| 42 | 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 |
| 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 |