

Yoshio Okiyama

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	FMODB: The World's First Database of Quantum Mechanical Calculations for Biomacromolecules Based on the Fragment Molecular Orbital Method. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 777-794.	5.4	24
2	Statistical interaction analyses between SARS-CoV-2 main protease and inhibitor N3 by combining molecular dynamics simulation and fragment molecular orbital calculation. <i>Applied Physics Express</i> , 2021, 14, 027003.	2.4	12
3	Molecular recognition of SARS-CoV-2 spike glycoprotein: quantum chemical hot spot and epitope analyses. <i>Chemical Science</i> , 2021, 12, 4722-4739.	7.4	37
4	In silico modeling of PAX8's PPAR γ fusion protein in thyroid carcinoma: influence of structural perturbation by fusion on ligand-binding affinity. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 629-642.	2.9	0
5	Dynamic Cooperativity of Ligand-Residue Interactions Evaluated with the Fragment Molecular Orbital Method. <i>Journal of Physical Chemistry B</i> , 2021, 125, 6501-6512.	2.6	17
6	Fragment Molecular Orbital Based Interaction Analyses on COVID-19 Main Protease's Inhibitor N3 Complex (PDB ID: 6LU7). <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3593-3602.	5.4	84
7	Fragment Molecular Orbital Calculations with Implicit Solvent Based on the Poisson-Boltzmann Equation: II. Protein and Its Ligand-Binding System Studies. <i>Journal of Physical Chemistry B</i> , 2019, 123, 957-973.	2.6	46
8	Fragment Molecular Orbital Calculations with Implicit Solvent Based on the Poisson-Boltzmann Equation: Implementation and DNA Study. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4457-4471.	2.6	35
9	Towards good correlation between fragment molecular orbital interaction energies and experimental IC ₅₀ for ligand binding: A case study of p38 MAP kinase. <i>Computational and Structural Biotechnology Journal</i> , 2018, 16, 421-434.	4.1	22