Yoshio Okiyama

List of Publications by Year
in descending order

9	277	1163117 8	1588992 8
papers	citations	h-index	g-index

9	9	9	227
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Fragment Molecular Orbital Based Interaction Analyses on COVID-19 Main Protease â˜ Inhibitor N3 Complex (PDB ID: 6LU7). Journal of Chemical Information and Modeling, 2020, 60, 3593-3602.	5.4	84
2	Fragment Molecular Orbital Calculations with Implicit Solvent Based on the Poissonâ€“Boltzmann Equation: II. Protein and Its Ligand-Binding System Studies. Journal of Physical Chemistry B, 2019, 123, 957-973.	2.6	46
3	Molecular recognition of SARS-CoV-2 spike glycoprotein: quantum chemical hot spot and epitope analyses. Chemical Science, 2021, 12, 4722-4739.	7.4	37
4	Fragment Molecular Orbital Calculations with Implicit Solvent Based on the Poissonâ€“Boltzmann Equation: Implementation and DNA Study. Journal of Physical Chemistry B, 2018, 122, 4457-4471.	2.6	35
5	FMODB: The Worldâ€™s First Database of Quantum Mechanical Calculations for Biomacromolecules Based on the Fragment Molecular Orbital Method. Journal of Chemical Information and Modeling, 2021, 61, 777-794.	5.4	24
6	Towards good correlation between fragment molecular orbital interaction energies and experimental IC50 for ligand binding: A case study of p38 MAP kinase. Computational and Structural Biotechnology Journal, 2018, 16, 421-434.	4.1	22
7	Dynamic Cooperativity of Ligandâ€“Residue Interactions Evaluated with the Fragment Molecular Orbital Method. Journal of Physical Chemistry B, 2021, 125, 6501-6512.	2.6	17
8	Statistical interaction analyses between SARS-CoV-2 main protease and inhibitor N3 by combining molecular dynamics simulation and fragment molecular orbital calculation. Applied Physics Express, 2021, 14, 027003.	2.4	12
9	In silico modeling of PAX8â€“PPARÎ³ fusion protein in thyroid carcinoma: influence of structural perturbation by fusion on ligand-binding affinity. Journal of Computer-Aided Molecular Design, 2021, 35, 629-642.	2.9	0