Tatsuya Nakano

List of Publications by Year
in descending order

31	3,542	331670 21	477307 29
papers	citations	h-index	g-index

32	32	32	1374
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Acceleration of Environmental Electrostatic Potential Using Cholesky Decomposition with Adaptive Metric (CDAM) for Fragment Molecular Orbital (FMO) Method. Bulletin of the Chemical Society of Japan, 2021, 94, 91-96.	3.2	1
2	The ABINIT-MP Program. , 2021, , 53-67.		10
3	How to Perform FMO Calculation in Drug Discovery. , 2021, , 93-125.		7
4	Fragmentation at sp 2 carbon atoms in fragment molecular orbital method. Journal of Computational Chemistry, 2020, 41, 1416-1420.	3.3	4
5	Development Status of ABINIT-MP in 2020. Journal of Computer Chemistry Japan, 2020, 19, 142-145.	0.1	3
6	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
7	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
8	Accuracy of the fragment molecular orbital (FMO) calculations for DNA: Total energy, molecular orbital, and inter-fragment interaction energy. Computational and Theoretical Chemistry, 2014, 1034, 7-16.	2.5	16
9	Three- and four-body corrected fragment molecular orbital calculations with a novel subdividing fragmentation method applicable to structure-based drug design. Journal of Molecular Graphics and Modelling, 2013, 41, 31-42.	2.4	48
10	Development of the four-body corrected fragment molecular orbital (FMO4) method. Chemical Physics Letters, 2012, 523, 128-133.	2.6	56
11	Antigenâ€“antibody interactions of influenza virus hemagglutinin revealed by the fragment molecular orbital calculation. Theoretical Chemistry Accounts, 2011, 130, 1197-1202.	1.4	16
12	Acceleration of fragment molecular orbital calculations with Cholesky decomposition approach. Chemical Physics Letters, 2010, 490, 84-89.	2.6	51
13	Incorporation of solvation effects into the fragment molecular orbital calculations with the Poissonâ€“Boltzmann equation. Chemical Physics Letters, 2010, 500, 116-119.	2.6	47
14	Does Amination of Formaldehyde Proceed Through a Zwitterionic Intermediate in Water? Fragment Molecular Orbital Molecular Dynamics Simulations by Using Constraint Dynamics. Chemistry - A European Journal, 2010, 16, 6430-6433.	3.3	21
15	Fragment molecular orbital (FMO) study on stabilization mechanism of neuro-oncological ventral antigen (NOVA)â€“RNA complex system. Computational and Theoretical Chemistry, 2010, 962, 45-55.	1.5	18
16	Fragment Molecular Orbital methodâ€based Molecular Dynamics (FMOâ€MD) as a simulator for chemical reactions in explicit solvation. Journal of Computational Chemistry, 2009, 30, 40-50.	3.3	57
17	Fragment molecular orbital-based molecular dynamics (FMO-MD), a quantum simulation tool for large molecular systems. Computational and Theoretical Chemistry, 2009, 898, 2-7.	1.5	59
18	Application of the fragment molecular orbital method for determination of atomic charges on polypeptides. II. Towards an improvement of force fields used for classical molecular dynamics simulations. Chemical Physics Letters, 2009, 467, 417-423.	2.6	42

#	Article	IF	Citations
19	Large scale FMO-MP2 calculations on a massively parallel-vector computer. Chemical Physics Letters, 2008, 457, 396-403.	2.6	113
20	How Does an S_N2 Reaction Take Place in Solution? Full Ab Initio MD Simulations for the Hydrolysis of the Methyl Diazonium Ion. Journal of the American Chemical Society, 2008, 130, 2396-2397.	13.7	71
21	DNA and Estrogen Receptor Interaction Revealed by Fragment Molecular Orbital Calculations. Journal of Physical Chemistry B, 2007, 111, 9621-9627.	2.6	43
22	Application of the fragment molecular orbital method for determination of atomic charges on polypeptides. Chemical Physics Letters, 2007, 449, 329-335.	2.6	36
23	Visualization analysis of inter-fragment interaction energies of CRPâ€“cAMPâ€“DNA complex based on the fragment molecular orbital method. Biophysical Chemistry, 2007, 130, 1-9.	2.8	47
24	VISCANA:Â Visualized Cluster Analysis of Proteinâ^'Ligand Interaction Based on the ab Initio Fragment Molecular Orbital Method for Virtual Ligand Screening. Journal of Chemical Information and Modeling, 2006, 46, 221-230.	5.4	127
25	Developments and applications of ABINIT-MP software based on the fragment molecular orbital method. , 2006, , 39-52.		36
26	Ab initio quantum mechanical study of the binding energies of human estrogen receptor ? with its ligands: An application of fragment molecular orbital method. Journal of Computational Chemistry, 2005, 26, 1-10.	3.3	132
27	Fragment molecular orbital method: use of approximate electrostatic potential. Chemical Physics Letters, 2002, 351, 475-480.	2.6	395
28	Fragment molecular orbital method: analytical energy gradients. Chemical Physics Letters, 2001, 336, 163-170.	2.6	197
29	Fragment molecular orbital method: application to polypeptides. Chemical Physics Letters, 2000, 318, 614-618.	2.6	333
30	Fragment molecular orbital method: an approximate computational method for large molecules. Chemical Physics Letters, 1999, 313, 701-706.	2.6	1,189
31	Pair interaction molecular orbital method: an approximate computational method for molecular interactions. Chemical Physics Letters, 1999, 312, 319-324.	2.6	271