Noriyuki Kurita

List of Publications by Year
in descending order

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70	395	933447	996975
papers	citations	10 h-index	15 g-index

72	72	72	375
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	Difference in dimer conformation between amyloid-Î²(1â€“42) and (1â€“43) proteins: Replica exchange molecular dynamics simulations in water. Chemical Physics Letters, 2014, 595-596, 242-249.	2.6	19
3	Stable conformation of full-length amyloid-Î² (1â€“42) monomer in water: Replica exchange molecular dynamics and ab initio molecular orbital simulations. Chemical Physics Letters, 2013, 577, 131-137.	2.6	17
4	Specific interactions between vitamin-D receptor and its ligands: Ab initio molecular orbital calculations in water. Journal of Steroid Biochemistry and Molecular Biology, 2017, 171, 75-79.	2.5	15
5	Ligand chirality can affect histidine protonation of vitamin-D receptor: ab initio molecular orbital calculations in water. Journal of Steroid Biochemistry and Molecular Biology, 2019, 186, 89-95.	2.5	15
6	Specific interactions between androgen receptor and its ligand: ab initio molecular orbital calculations in water. Journal of Molecular Graphics and Modelling, 2017, 75, 383-389.	2.4	13
7	Proposal of potent inhibitors for vitamin-D receptor based on ab initio fragment molecular orbital calculations. Journal of Molecular Graphics and Modelling, 2018, 80, 320-326.	2.4	13
8	Specific interactions between tau protein and curcumin derivatives: Molecular docking and ab initio molecular orbital simulations. Journal of Molecular Graphics and Modelling, 2020, 98, 107611.	2.4	13
9	Proposal of novel natural inhibitors of severe acute respiratory syndrome coronavirus 2 main protease: Molecular docking and ab initio fragment molecular orbital calculations. Biophysical Chemistry, 2021, 275, 106608.	2.8	13
10	A combined simulation with ab initio MO and classical vibrational analysis on the specific interactions between thermolysin and dipeptide ligands. Chemical Physics Letters, 2009, 479, 290-295.	2.6	11
11	Specific interactions between aryl hydrocarbon receptor and dioxin congeners: Ab initio fragment molecular orbital calculations. Journal of Molecular Graphics and Modelling, 2010, 29, 197-205.	2.4	11
12	Specific interactions and binding free energies between thermolysin and dipeptides: Molecular simulations combined with Ab initio molecular orbital and classical vibrational analysis. Journal of Computational Chemistry, 2011, 32, 3047-3057.	3.3	11
13	The effects of amino-acid mutations on specific interactions between urokinase-type plasminogen activator and its receptor: Ab initio molecular orbital calculations. Journal of Molecular Graphics and Modelling, 2011, 29, 975-984.	2.4	10
14	Effect of D23N mutation on the dimer conformation of amyloid Î²-proteins: Ab initio molecular simulations in water. Journal of Molecular Graphics and Modelling, 2014, 50, 113-124.	2.4	9
15	Attacking mechanism of hydroxyl radical to DNA base-pair: density functional study in vacuum and in water. Journal of Biomolecular Structure and Dynamics, 2015, 33, 158-166.	3.5	9
16	A coarse grained molecular dynamics study on the structure and stability of small-sized liposomes. Molecular Simulation, 2016, 42, 122-130.	2.0	9
17	Proposal of therapeutic curcumin derivatives for Alzheimerâ€™s disease based on ab initio molecular simulations. Chemical Physics Letters, 2020, 738, 136883.	2.6	9
18	Specific interactions and binding energies between thermolysin and potent inhibitors: Molecular simulations based on ab initio molecular orbital method. Journal of Molecular Graphics and Modelling, 2012, 33, 1-11.	2.4	8

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19	DFT Study on Reaction Mechanism of DNA Base Pair with Hydroxyl Radical. Journal of Modern Physics, 2013, 04, 442-451.	0.6	8
20	Ab initio molecular simulations for proposing potent inhibitors to butyrylcholinesterases. Journal of Molecular Graphics and Modelling, 2014, 54, 54-61.	2.4	8
21	Specific interactions between amyloid-Î² peptide and curcumin derivatives: Ab initio molecular simulations. Chemical Physics Letters, 2015, 633, 139-145.	2.6	8
22	Binding sites of Zantrin inhibitors to the bacterial cell division protein FtsZ: Molecular docking and ab initio molecular orbital calculations. Chemical Physics, 2020, 530, 110603.	1.9	8
23	Ab initio molecular orbital calculations on specific interactions between urokinase-type plasminogen activator and its receptor. Journal of Molecular Graphics and Modelling, 2009, 28, 46-53.	2.4	7
24	Specific interactions between amyloid-Î² peptides in an amyloid-Î² hexamer with three-fold symmetry: Ab initio fragment molecular orbital calculations in water. Chemical Physics Letters, 2017, 672, 13-20.	2.6	7
25	Single-molecule junction spontaneously restored by DNA zipper. Nature Communications, 2021, 12, 5762.	12.8	7
26	Change in specific interactions between lactose repressor protein and DNA induced by ligand binding: molecular dynamics and molecular orbital calculations. Molecular Simulation, 2016, 42, 242-256.	2.0	6
27	Specific interactions between mycobacterial FtsZ protein and curcumin derivatives: Molecular docking and ab initio molecular simulations. Chemical Physics Letters, 2018, 692, 166-173.	2.6	6
28	Structural change of retinoic-acid receptor-related orphan receptor induced by binding of inverse-agonist: Molecular dynamics and ab initio molecular orbital simulations. Computational and Structural Biotechnology Journal, 2020, 18, 1676-1685.	4.1	6
29	Specific interactions between vitamin D receptor and ligand depending on its chirality: ab initio fragment molecular orbital calculations. Chem-Bio Informatics Journal, 2018, 18, 32-43.	0.3	6
30	Specific interactions between lactose repressor protein and DNA affected by ligand binding: Ab initio molecular orbital calculations. Journal of Computational Chemistry, 2011, 32, 1661-1670.	3.3	5
31	Structures and electronic properties of metal organic frameworks: DFT and ab initio FMO calculations for model systems. Chemical Physics Letters, 2014, 612, 295-301.	2.6	5
32	Specific interactions between zinc metalloproteinase and its inhibitors: Ab initio fragment molecular orbital calculations. Journal of Molecular Graphics and Modelling, 2017, 75, 277-286.	2.4	5
33	Change in binding states between catabolite activating protein and DNA induced by ligand-binding: molecular dynamics and ab initio fragment molecular orbital calculations. Journal of Molecular Modeling, 2019, 25, 192.	1.8	5
34	The effects of vitronectin on specific interactions between urokinase-type plasminogen activator and its receptor:ab initiomolecular orbital calculations. Molecular Simulation, 2013, 39, 769-779.	2.0	4
35	Binding affinity between AhR and exogenous/endogenous ligands: molecular simulations and biological experiment. Molecular Simulation, 2015, 41, 555-563.	2.0	4
36	Influence of solvating water molecules on the attacking mechanisms of OH-radical to DNA base pairs: DFT calculations in explicit waters. Structural Chemistry, 2016, 27, 1793-1806.	2.0	4

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37	Specific interactions between 2-trans enoyl-acyl carrier protein reductase and its ligand: Protein-ligand docking and ab initio fragment molecular orbital calculations. Journal of Molecular Graphics and Modelling, 2019, 88, 299-308.	2.4	4
38	Protonation states of central amino acids in a zinc metalloprotease complexed with inhibitor: Molecular mechanics optimizations and ab initio molecular orbital calculations. Biophysical Chemistry, 2020, 261, 106368.	2.8	4
39	Electronic Properties for Medicine Inhibiting Cancer Metastasis (1) : Molecular Orbital Calculations for Physiological Substance Bikunin. Journal of Computer Aided Chemistry, 2004, 5, 62-69.	0.3	4
40	Electronic Properties for Medicine Inhibiting Cancer Metastasis (2) : Molecular Mechanics and Molecular Orbital Calculations for Urokinase. Journal of Computer Aided Chemistry, 2004, 5, 70-78.	0.3	4
41	Ab initio molecular simulations on specific interactions between amyloid beta and monosaccharides. Chemical Physics Letters, 2012, 547, 89-96.	2.6	3
42	Proposal for novel curcumin derivatives as potent inhibitors against Alzheimerâ€™s disease: Ab initio molecular simulations on the specific interactions between amyloid-beta peptide and curcumin. Chemical Physics Letters, 2017, 685, 482-489.	2.6	3
43	Binding properties between curcumin and malarial tubulin: molecular-docking and ab initio fragment molecular orbital calculations. Chem-Bio Informatics Journal, 2018, 18, 44-57.	0.3	3
44	Binding energy between lactose repressor protein and DNA: semiempirical molecular orbital calculations. Journal of Computer Aided Chemistry, 2003, 4, 35-41.	0.3	3
45	Analysis of Cancer Invasion Mechanism by Cellular Simulation. Journal of Computer Aided Chemistry, 2007, 8, 75-84.	0.3	3
46	STRUCTURES AND ELECTRONIC PROPERTIES OF MONOMER, DIMER AND TETRAMER OF LACTOSE REPRESSOR PROTEIN: MOLECULAR MECHANICS, MOLECULAR DYNAMICS, MOLECULAR ORBITAL AND CHARGE EQUILIBRATION CALCULATIONS. Journal of Theoretical and Computational Chemistry, 2006, 05, 59-74.	1.8	2
47	Ab initio fragment molecular orbital calculations on specific interactions between aryl hydrocarbon receptor and dioxin. International Journal of Quantum Chemistry, 2012, 112, 289-299.	2.0	2
48	A proposal of potent inhibitor for cancer metastasis blocking the pocket of urokinase receptor: ab initio molecular simulations. Journal of Physics: Conference Series, 2013, 433, 012034.	0.4	2
49	Ab initio molecular simulations for proposing novel peptide inhibitors blocking the ligand-binding pocket of urokinase receptor. Journal of Molecular Modeling, 2014, 20, 2292.	1.8	2
50	A novel peptide blocking cancer cell invasion by structure-based drug design. Biomedical Reports, 2017, 7, 221-225.	2.0	2
51	Effect of Zn ion on the structure and electronic states of AÎ² nonamer: molecular dynamics and ab initio molecular orbital calculations. Molecular Simulation, 2019, 45, 706-715.	2.0	2
52	Design of galardine analogs as putative psudolysin inhibitors based on ab initio fragment molecular orbital calculations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3307-3317.	3.5	2
53	Molecular Mechanics and Molecular Orbital Simulations on The Specific Interactions between Lactose Repressor Protein and Its Inducer and Anti-Inducer Molecules. Journal of Computer Aided Chemistry, 2008, 9, 17-29.	0.3	2
54	Proposal of selective inhibitor for bacterial zinc metalloprotease: Molecular mechanics and ab initio molecular orbital calculations. Journal of Molecular Graphics and Modelling, 2022, 110, 108047.	2.4	2

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55	A combined Greenâ€™s function/density-functional theory study of electrical conducting properties of solvated single molecules tethered to Au electrodes. Chemical Physics Letters, 2012, 521, 39-44.	2.6	1
56	Ab initio molecular simulations on specific interactions between amyloid-Î² peptide and new curcumin derivatives. , 2016, , .		1
57	Ab initio fragment molecular orbital calculations on the specific interactions between amyloid-Î² peptides in an in vivo amyloid-Î² fibril. , 2016, , .		1
58	Molecular dynamics and ab initio FMO calculations on the effect of water molecules on the interactions between androgen receptor and its ligand and cofactor. , 2016, , .		1
59	Proposal of Potent Inhibitors for a Bacterial Cell Division Protein FtsZ: Molecular Simulations Based on Molecular Docking and ab Initio Molecular Orbital Calculations. Antibiotics, 2020, 9, 846.	3.7	1
60	Proposal of novel inhibitors for vitamin-D receptor: Molecular docking, molecular mechanics and ab initio molecular orbital simulations. Biophysical Chemistry, 2021, 270, 106540.	2.8	1
61	Proposal of novel potent inhibitors against androgen receptor based on ab initio molecular orbital calculations. Journal of Molecular Graphics and Modelling, 2021, 105, 107873.	2.4	1
62	FMO Drug Design Consortium. , 2021, , 127-181.		1
63	Ab initio molecular simulations on the binding properties between mycobacterial FtsZ and its inhibitor. , 2016, , .		0
64	Effect of cofactor-binding on the specific interactions between androgen receptor and its ligand: Ab initio molecular simulations. , 2016, , .		0
65	Ab initio molecular simulations based on FMO method for proposing potent inhibitors to reverse transcriptase of HIV. , 2016, , .		0
66	Specific interactions between M. tuberculosis CYP130 and its inhibitors: Molecular simulations using ab initio fragment molecular orbital method. , 2016, , .		0
67	Molecular dynamics and ab initio molecular orbital calculations on conformational change of amyloid-ĀŸ monomers in an in vivo amyloid-ĀŸ nonamer. , 2017, , .		0
68	Drug Discovery Screening by Combination of X-ray Crystal Structure Analysis and FMO Calculation. , 2021, , 253-265.		0
69	Specific interactions between the alkaline protease of P. aeruginosa and its natural peptide inhibitor: ab initio molecular simulations. Journal of Molecular Modeling, 2022, 28, 10.	1.8	0
70	Water molecule-mediated selective inhibition of bacterial zinc metalloproteinases by non-hydroxamate compounds: Ab initio molecular simulations. Journal of Molecular Graphics and Modelling, 2022, 114, 108200.	2.4	0