Hiroaki Tokiwa

List of Publications by Year in descending order

60	1,142	393982	433756
papers	citations	19 h-index	31 g-index

63	63	63	1255
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Parallelized integral-direct CIS(D) calculations with multilayer fragment molecular orbital scheme. Theoretical Chemistry Accounts, 2007, 117, 541-553.	0.5	71
2	Regiocomplementary Cycloaddition Reactions of Boryl- and Silylbenzynes with 1,3-Dipoles: Selective Synthesis of Benzo-Fused Azole Derivatives. Journal of Organic Chemistry, 2013, 78, 2965-2983.	1.7	70
3	Crystal Structures of Rat Vitamin D Receptor Bound to Adamantyl Vitamin D Analogs: Structural Basis for Vitamin D Receptor Antagonism and Partial Agonism. Journal of Medicinal Chemistry, 2008, 51, 5320-5329.	2.9	65
4	Fragment interaction analysis based on local MP2. Theoretical Chemistry Accounts, 2007, 118, 937-945.	0.5	62
5	Comparative Binding Analysis of Dipeptidyl Peptidase IV (DPP-4) with Antidiabetic Drugs â€“ An Ab Initio Fragment Molecular Orbital Study. PLoS ONE, 2016, 11, e0166275.	1.1	59
6	Vitamin D Receptor:â€‰ Ligand Recognition and Allosteric Network. Journal of Medicinal Chemistry, 2006, 49, 1313-1324.	2.9	54
7	Molecular association model of PPARÎ± and its new specific and efficient ligand, pemafibrate: Structural basis for SPPARMÎ±. Biochemical and Biophysical Research Communications, 2018, 499, 239-245.	1.0	47
8	Hepatocyte ELOVL Fatty Acid Elongase 6 Determines Ceramide Acylâ€Chain Length and Hepatic Insulin Sensitivity in Mice. Hepatology, 2020, 71, 1609-1625.	3.6	44
9	Functions of key residues in the ligand-binding pocket of vitamin D receptor: Fragment molecular orbitalâ€“interfragment interaction energy analysis. Chemical Physics Letters, 2006, 420, 465-468.	1.2	32
10	Generation of 3-borylbenzynes, their regioselective Dielsâ€“Alder reactions, and theoretical analysis. Tetrahedron, 2013, 69, 4338-4352.	1.0	32
11	Electron Affinity for the Most Toxic 2,3,7,8-Tetrachlorodibenzo-p-dioxin (TCDD):â€‰ A Density Functional Theory Study. Journal of Physical Chemistry A, 2000, 104, 7068-7072.	1.1	25
12	Interactions between 1Î±,25(OH)2D3 and residues in the ligand-binding pocket of the vitamin D receptor: A correlated fragment molecular orbital study. Journal of Steroid Biochemistry and Molecular Biology, 2010, 121, 63-67.	1.2	25
13	Ab initio fragment molecular orbital studies of influenza virus hemagglutininâ€“sialosaccharide complexes toward chemical clarification about the virus host range determination. Glycoconjugate Journal, 2008, 25, 805-815.	1.4	24
14	Protein Residue Networks from Energetic and Geometric Data: Are They Identical?. Journal of Chemical Theory and Computation, 2018, 14, 6623-6631.	2.3	24
15	Animal morbilliviruses and their cross-species transmission potential. Current Opinion in Virology, 2020, 41, 38-45.	2.6	24
16	Catalytic preference of Salmonella typhimurium LT2 sialidase for Nâ€acetylneuraminic acid residues over Nâ€glycolylneuraminic acid residues. FEBS Open Bio, 2013, 3, 231-236.	1.0	23
17	Combination of Triple Bond and Adamantane Ring on the Vitamin D Side Chain Produced Partial Agonists for Vitamin D Receptor. Journal of Medicinal Chemistry, 2014, 57, 4073-4087.	2.9	23
18	A Novel Potent and Highly Specific Inhibitor against Influenza Viral N1â€“N9 Neuraminidases: Insight into Neuraminidaseâ€“Inhibitor Interactions. Journal of Medicinal Chemistry, 2016, 59, 4563-4577.	2.9	23

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19	Flexible ligand recognition of peroxisome proliferator-activated receptor-Î³ (PPARÎ³). Bioorganic and Medicinal Chemistry Letters, 2010, 20, 3344-3347.	1.0	21
20	Origin of Stereoselectivity and Substrate/Ligand Recognition in an FAD-Dependent R-Selective Amine Oxidase. Journal of Physical Chemistry B, 2016, 120, 10736-10743.	1.2	20
21	Elucidation of Molecular Mechanism of a Selective PPARÎ± Modulator, Pemafibrate, through Combinational Approaches of X-ray Crystallography, Thermodynamic Analysis, and First-Principle Calculations. International Journal of Molecular Sciences, 2020, 21, 361.	1.8	20
22	Mechanistic Insight into Weak Baseâ€Catalyzed Generation of Carbon Monoxide from Phenyl Formate and Its Application to Catalytic Carbonylation at Room Temperature without Use of External Carbon Monoxide Gas. Advanced Synthesis and Catalysis, 2017, 359, 3592-3601.	2.1	19
23	Could London Dispersion Force Control Regioselective (2 + 2) Cyclodimerizations of Benzynes? YES: Application to the Synthesis of Helical Biphenylenes. Journal of the American Chemical Society, 2021, 143, 10853-10859.	6.6	19
24	Binding of NAD+ and l-Threonine Induces Stepwise Structural and Flexibility Changes in Cupriavidus necator l-Threonine Dehydrogenase. Journal of Biological Chemistry, 2014, 289, 10445-10454.	1.6	18
25	RXR Partial Agonist Produced by Side Chain Repositioning of Alkoxy RXR Full Agonist Retains Antitype 2 Diabetes Activity without the Adverse Effects. Journal of Medicinal Chemistry, 2015, 58, 912-926.	2.9	18
26	3-(Triflyloxy)benzynes Enable the Regiocontrolled Cycloaddition of Cyclic Ureas to Synthesize 1,4-Benzodiazepine Derivatives. Synlett, 2018, 29, 943-948.	1.0	18
27	Benchmark Analysis of Native and Artificial NAD⁺-Dependent Enzymes Generated by a Sequence-Based Design Method with or without Phylogenetic Data. Biochemistry, 2018, 57, 3722-3732.	1.2	18
28	Isotope Effect in Hydrogen/Deuterium-absorbing Pd Nanoparticles Revealed by X-ray Powder Diffraction and by a Multi-component MO Method. Journal of the Physical Society of Japan, 2004, 73, 1775-1780.	0.7	17
29	Experimental and Theoretical Studies on Regiocontrol of Benzyne Reactions Using Silyl and Boryl Directing Groups. Yuki Gosei Kagaku Kyokaishi/Journal of Synthetic Organic Chemistry, 2012, 70, 1123-1133.	0.0	17
30	Ab initio fragment molecular orbital study of ligand binding to human progesterone receptor ligand-binding domain. Naunyn-Schmiedeberg's Archives of Pharmacology, 2008, 377, 607-615.	1.4	15
31	Structural and computational analysis of peptide recognition mechanism of class-C type penicillin binding protein, alkaline D-peptidase from Bacillus cereus DF4-B. Scientific Reports, 2015, 5, 13836.	1.6	15
32	Synthetic Small Molecules Derived from Natural Vitamin K Homologues that Induce Selective Neuronal Differentiation of Neuronal Progenitor Cells. Journal of Medicinal Chemistry, 2015, 58, 7088-7092.	2.9	14
33	First-Principle Calculation on Isotope Effect in KH 2 PO 4 and KD 2 PO 4 of Hydrogen-Bonded Dielectric Materials. Approach with Dynamic Extended Molecular Orbital Method. Ferroelectrics, 2002, 268, 3-9.	0.3	13
34	Synthesis, Biological Activities, and X-ray Crystal Structural Analysis of 25-Hydroxy-25(or) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 147 Td (58, 9510-9521.	2.9	13
35	Competitive Binding Assay with an Umbelliferone-Based Fluorescent Rexinoid for Retinoid X Receptor Ligand Screening. Journal of Medicinal Chemistry, 2019, 62, 8809-8818.	2.9	13
36	Total Synthesis of Termicalcicolanone A via Organocatalysis and Regioselective Claisen Rearrangement. Organic Letters, 2019, 21, 2777-2781.	2.4	13

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37	Development of an Analysis Toolkit, AnalysisFMO, to Visualize Interaction Energies Generated by Fragment Molecular Orbital Calculations. Journal of Chemical Information and Modeling, 2019, 59, 25-30.	2.5	13
38	Anti-MRSA activity of isoplagiochin-type macrocyclic bis(bibenzyl)s is mediated through cell membrane damage. Bioorganic and Medicinal Chemistry, 2015, 23, 3309-3316.	1.4	12
39	The transcriptional corepressor CtBP2 serves as a metabolite sensor orchestrating hepatic glucose and lipid homeostasis. Nature Communications, 2021, 12, 6315.	5.8	12
40	Amino acid substitutions contributing to Î±2,6â€sialic acid linkage binding specificity of human parainfluenza virus type 3 hemagglutininâ€“neuraminidase. FEBS Letters, 2015, 589, 1278-1282.	1.3	11
41	Product Release Mechanism Associated with Structural Changes in Monomeric l-Threonine 3-Dehydrogenase. Biochemistry, 2017, 56, 5758-5770.	1.2	11
42	Ligand-dependent conformation change reflects steric structure and interactions of a vitamin D receptor/ligand complex: A fragment molecular orbital study. Journal of Steroid Biochemistry and Molecular Biology, 2010, 121, 56-59.	1.2	9
43	Origin of the inhibitory activity of 4-O-substituted sialic derivatives of human parainfluenza virus. Glycoconjugate Journal, 2012, 29, 231-237.	1.4	7
44	25S-Adamantyl-23-yne-26,27-dinor-1Î±,25-dihydroxyvitamin D₃: Synthesis, Tissue Selective Biological Activities, and X-ray Crystal Structural Analysis of Its Vitamin D Receptor Complex. Journal of Medicinal Chemistry, 2018, 61, 6658-6673.	2.9	7
45	Computational design of a sulfoglucuronide derivative fitting into a hydrophobic pocket of dengue virus E protein. Biochemical and Biophysical Research Communications, 2014, 449, 32-37.	1.0	6
46	Theoretical study of N2O adsorption on clean and partially oxidized Si(1 0 0)-(2 Ã— 1) small clusters. Chemical Physics Letters, 2007, 436, 263-267.	1.2	5
47	Dual conformation of the ligand induces the partial agonistic activity of retinoid X receptor Î± (<scp>RXR</scp>Î±). FEBS Letters, 2019, 593, 242-250.	1.3	5
48	Measles Virus Hemagglutinin Protein Establishes a Specific Interaction With the Extreme N-Terminal Region of Human Signaling Lymphocytic Activation Molecule to Enhance Infection. Frontiers in Microbiology, 2020, 11, 1830.	1.5	4
49	Computational Analysis Reveals a Critical Point Mutation in the N-Terminal Region of the Signaling Lymphocytic Activation Molecule Responsible for the Cross-Species Infection with Canine Distemper Virus. Molecules, 2021, 26, 1262.	1.7	4
50	Molecular dynamics study-guided identification of cyclic amine structures as novel hydrophobic tail components of hPPARÎ³ agonists. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 4001-4005.	1.0	3
51	First-Principle Calculation on Isotope Effect in KH 2 PO 4 and KD 2 PO 4 of Hydrogen-Bonded Dielectric Materials. Approach with Dynamic Extended Molecular Orbital Method. , 0, .		3
52	InOH:â€‰ A Quantum Chemical Study. Journal of Physical Chemistry A, 1999, 103, 4085-4088.	1.1	2
53	Hybrid-DFT study for the initial oxidation steps on silicon cluster surface. Applied Surface Science, 2008, 254, 7909-7912.	3.1	0
54	Elucidating the Efficacy of Clinical Drugs Using FMO. , 2021, , 323-339.		0

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55	AnalysisFMO Toolkit: A PyMOL Plugin for 3D-Visualization of Interaction Energies in Proteins (3D-VIEP) Calculated by the FMO Method. , 2021, , 357-370.		0
56	Theoretical Study of NO Adsorption and Decomposition on Si(100) Surfaces. E-Journal of Surface Science and Nanotechnology, 2006, 4, 624-629.	0.1	0
57	What is the origin of partial agonist activity of CBtâ€PMN for hRXRÎ±?. FASEB Journal, 2018, 32, 530.22.	0.2	0
58	How to design artificial protein surpassing native enzyme function ~ Design and multidisciplinary analysis of artificial Lâ€threonine 3â€dehydrogenase ~. FASEB Journal, 2018, 32, 798.4.	0.2	0
59	Computational design and molecular mechanism in oligomerization of Câ€terminal binding protein 2. FASEB Journal, 2018, 32, 798.22.	0.2	0
60	Discovery of novel monomeric Lâ€threonine 3â€dehydrogenase and elucidation of product release mechanism. FASEB Journal, 2018, 32, 796.14.	0.2	0