Hiroaki Tokiwa

List of Publications by Year
in descending order

60	1,142	394286	434063
papers	citations	19 h-index	31 g-index

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

#	Article	IF	Citations
1	Elucidating the Efficacy of Clinical Drugs Using FMO. , 2021, , 323-339.		0
2	AnalysisFMO Toolkit: A PyMOL Plugin for 3D-Visualization of Interaction Energies in Proteins (3D-VIEP) Calculated by the FMO Method. , 2021, , 357-370.		0
3	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
4	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
5	The transcriptional corepressor CtBP2 serves as a metabolite sensor orchestrating hepatic glucose and lipid homeostasis. Nature Communications, 2021, 12, 6315.	5.8	12
6	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
7	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
8	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
9	Animal morbilliviruses and their cross-species transmission potential. Current Opinion in Virology, 2020, 41, 38-45.	2.6	24
10	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
11	Total Synthesis of Termicalcicolanone A via Organocatalysis and Regioselective Claisen Rearrangement. Organic Letters, 2019, 21, 2777-2781.	2.4	13
12	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
13	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
14	3-(Triflyloxy)benzynes Enable the Regiocontrolled Cycloaddition of Cyclic Ureas to Synthesize 1,4-Benzodiazepine Derivatives. Synlett, 2018, 29, 943-948.	1.0	18
15	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
16	Protein Residue Networks from Energetic and Geometric Data: Are They Identical?. Journal of Chemical Theory and Computation, 2018, 14, 6623-6631.	2.3	24
17	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
18	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

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19	What is the origin of partial agonist activity of CBtâ€PMN for hRXRÎ±?. FASEB Journal, 2018, 32, 530.22.	0.2	0
20	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
21	Computational design and molecular mechanism in oligomerization of Câ€terminal binding protein 2. FASEB Journal, 2018, 32, 798.22.	0.2	0
22	Discovery of novel monomeric Lâ€threonine 3â€dehydrogenase and elucidation of product release mechanism. FASEB Journal, 2018, 32, 796.14.	0.2	0
23	Product Release Mechanism Associated with Structural Changes in Monomeric l-Threonine 3-Dehydrogenase. Biochemistry, 2017, 56, 5758-5770.	1.2	11
24	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
25	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
26	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
27	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
28	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
29	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
30	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
31	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
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	Synthesis, Biological Activities, and X-ray Crystal Structural Analysis of 25-Hydroxy-25(or) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 58, 9510-9521.	2.9	13
34	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
35	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
36	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

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37	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
38	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
39	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
40	Generation of 3-borylbenzynes, their regioselective Dielsâ€“Alder reactions, and theoretical analysis. Tetrahedron, 2013, 69, 4338-4352.	1.0	32
41	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
42	Origin of the inhibitory activity of 4-O-substituted sialic derivatives of human parainfluenza virus. Glycoconjugate Journal, 2012, 29, 231-237.	1.4	7
43	Flexible ligand recognition of peroxisome proliferator-activated receptor-Î³ (PPARÎ³). Bioorganic and Medicinal Chemistry Letters, 2010, 20, 3344-3347.	1.0	21
44	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
45	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
46	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
47	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
48	Hybrid-DFT study for the initial oxidation steps on silicon cluster surface. Applied Surface Science, 2008, 254, 7909-7912.	3.1	0
49	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
50	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
51	Parallelized integral-direct CIS(D) calculations with multilayer fragment molecular orbital scheme. Theoretical Chemistry Accounts, 2007, 117, 541-553.	0.5	71
52	Fragment interaction analysis based on local MP2. Theoretical Chemistry Accounts, 2007, 118, 937-945.	0.5	62
53	Vitamin D Receptor:â€‰ Ligand Recognition and Allosteric Network. Journal of Medicinal Chemistry, 2006, 49, 1313-1324.	2.9	54
54	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

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55	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
56	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
57	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
58	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
59	InOH:â€‰ A Quantum Chemical Study. Journal of Physical Chemistry A, 1999, 103, 4085-4088.	1.1	2
60	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