Yusuke Kanematsu

List of Publications by Year
in descending order

23	299	933447 10	888059 17
papers	citations	h-index	g-index

23	23	23	404
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Capturing an initial intermediate during the P450nor enzymatic reaction using time-resolved XFEL crystallography and caged-substrate. Nature Communications, 2017, 8, 1585.	12.8	74
2	Theoretical study of the H/D isotope effect on phase transition of hydrogen-bonded organic conductor Îº-H₃(Cat-EDT-TTF)₂. Physical Chemistry Chemical Physics, 2016, 18, 29673-29680.	2.8	26
3	Theoretical analysis of geometry and NMR isotope shift in hydrogen-bonding center of photoactive yellow protein by combination of multicomponent quantum mechanics and ONIOM scheme. Journal of Chemical Physics, 2014, 141, 185101.	3.0	22
4	Short-lived intermediate in N ₂ O generation by P450 NO reductase captured by time-resolved IR spectroscopy and XFEL crystallography. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	21
5	Development of multicomponent hybrid density functional theory with polarizable continuum model for the analysis of nuclear quantum effect and solvent effect on NMR chemical shift. Journal of Chemical Physics, 2014, 140, 164111.	3.0	16
6	Strong Hydrogen Bonds at the Interface between Proton-Donating and -Accepting Self-Assembled Monolayers on Au(111). Langmuir, 2018, 34, 2189-2197.	3.5	16
7	Computational study of distortion effect of Fe-porphyrin found as a biological active site. Japanese Journal of Applied Physics, 2020, 59, 010502.	1.5	14
8	Statistical and quantum-chemical analysis of the effect of heme porphyrin distortion in heme proteins: Differences between oxidoreductases and oxygen carrier proteins. Chemical Physics Letters, 2018, 710, 108-112.	2.6	13
9	Multicomponent DFT study of geometrical H/D isotope effect on hydrogen-bonded organic conductor, Îº-H 3 (Cat EDT-ST) 2. Chemical Physics Letters, 2017, 674, 168-172.	2.6	12
10	PyDISH: database and analysis tools for heme porphyrin distortion in heme proteins. Database: the Journal of Biological Databases and Curation, 2023, 2023, .	3.0	12
11	Performance Test of Multicomponent Quantum Mechanical Calculation with Polarizable Continuum Model for Proton Chemical Shift. Journal of Physical Chemistry A, 2015, 119, 4933-4938.	2.5	11
12	Global Analysis of Heme Proteins Elucidates the Correlation between Heme Distortion and the Heme-Binding Pocket. Journal of Chemical Information and Modeling, 2022, 62, 775-784.	5.4	10
13	Isotope effect on the circular dichroism spectrum of methyl Î±-D-glucopyranoside in aqueous solution. Scientific Reports, 2016, 5, 17900.	3.3	9
14	Applicability of Density Functional Tight Binding Method with Dispersion Correction to Investigate the Adsorption of Porphyrin/Porphycene Metal Complexes on Graphene. Chemistry Letters, 2017, 46, 51-52.	1.3	8
15	Structure of Heme-binding Pocket in Heme Protein is Generally Rigid and can be Predicted by AlphaFold2. Chemistry Letters, 2022, 51, 704-708.	1.3	8
16	Inverse Ubbelohde effect in the short hydrogen bond of photosystem II: Relation between H/D isotope effect and symmetry in potential energy profile. Journal of Computational Chemistry, 2016, 37, 2140-2145.	3.3	6
17	Vibrational analysis on the revised potential energy curve of the low-barrier hydrogen bond in photoactive yellow protein. Computational and Structural Biotechnology Journal, 2016, 14, 16-19.	4.1	6
18	A computational examination of the electric-field-induced proton transfer along the interface hydrogen bond between proton donating and accepting self-assembled monolayers. Chemical Physics Letters, 2020, 741, 137091.	2.6	5

#	Article	IF	Citations
19	Quantum Mechanics/Molecular Mechanics Study of the Sialyltransferase Reaction Mechanism. Biochemistry, 2016, 55, 5764-5771.	2.5	4
20	Hydrogen/Deuterium Transfer from Anisole to Methoxy Radicals: A Theoretical Study of a Deuterium-Labeled Drug Model. Journal of Physical Chemistry A, 2022, 126, 155-163.	2.5	3
21	Substrateâ€shielding and hydrolytic reaction in hydrolases. Proteins: Structure, Function and Bioinformatics, 2013, 81, 926-932.	2.6	1
22	H/D isotope effect between adsorbed water (H2O, D2O, and HDO) and H2O- and D2O-ice Ih(0Â0Â0Â1) basal surfaces based on the combined plane wave and localized basis set method. Applied Surface Science, 2021, 561, 150100.	6.1	1
23	Nuclear quantum effect and H/D isotope effect in excited state intramolecular proton transfer and electronâ€induced intramolecular proton transfer reactions in 8â€hydroxyquinoline. International Journal of Quantum Chemistry, 0, , .	2.0	1