Tomoki Nakayoshi

List of Publications by Year
in descending order

32 papers	258 citations	1040056 9 h-index	1058476 14 g-index
32 all docs	32 docs citations	32 times ranked	135 citing authors

#	Article	IF	Citations
1	Computational analysis of nonenzymatic deamidation of asparagine residues catalysed by acetic acid. Molecular Physics, 2021, 119, e1827176.	1.7	0
2	(S)-Erypoegin K, an isoflavone isolated from Erythrina poeppigiana, is a novel inhibitor of topoisomerase IIÎ±: Induction of G2 phase arrest in human gastric cancer cells. Bioorganic and Medicinal Chemistry, 2021, 30, 115904.	3.0	3
3	Molecular Mechanisms of Succinimide Formation from Aspartic Acid Residues Catalyzed by Two Water Molecules in the Aqueous Phase. International Journal of Molecular Sciences, 2021, 22, 509.	4.1	5
4	Functional Assessment of 12 Rare Allelic CYP2C9 Variants Identified in a Population of 4773 Japanese Individuals. Journal of Personalized Medicine, 2021, 11, 94.	2.5	7
5	Modification of the pH Dependence of Assembly of Yeast Cargo Receptor Emp47p Coiled-Coil Domains: Computational Design and Experimental Mutagenesis. Journal of Physical Chemistry B, 2021, 125, 2222-2230.	2.6	0
6	Functional Characterization of 21 Rare Allelic CYP1A2 Variants Identified in a Population of 4773 Japanese Individuals by Assessing Phenacetin O-Deethylation. Journal of Personalized Medicine, 2021, 11, 690.	2.5	5
7	Theoretical Studies on the Effect of Isomerized Aspartic Acid Residues on the Three-Dimensional Structures of Bovine Pancreatic Ribonucleases A. Biological and Pharmaceutical Bulletin, 2021, 44, 967-975.	1.4	1
8	Deciphering Structural Alterations Associated with Activity Reductions of Genetic Polymorphisms in Cytochrome P450 2A6 Using Molecular Dynamics Simulations. International Journal of Molecular Sciences, 2021, 22, 10119.	4.1	3
9	Effects of substituent pattern on the intracellular target of antiproliferative benzo[b]thiophenyl chromone derivatives. European Journal of Medicinal Chemistry, 2021, 222, 113578.	5.5	16
10	Molecular dynamics simulations for the proteinâ€“ligand complex structures obtained by computational docking studies using implicit or explicit solvents. Chemical Physics Letters, 2021, 781, 139022.	2.6	12
11	Functional Characterization of 40 CYP3A4 Variants by Assessing Midazolam 1â€²-Hydroxylation and Testosterone 6Î²-Hydroxylation. Drug Metabolism and Disposition, 2021, 49, 212-220.	3.3	20
12	Computational Analysis of the Mechanism of Nonenzymatic Peptide Bond Cleavage at the C-Terminal Side of an Asparagine Residue. ACS Omega, 2021, 6, 30078-30084.	3.5	4
13	Nonenzymatic Deamidation Mechanism on a Glutamine Residue with a C-Terminal Adjacent Glycine Residue: A Computational Mechanistic Study. AppliedChem, 2021, 1, 142-155.	1.0	2
14	CYP2D6 genotyping analysis and functional characterization of novel allelic variants in a Ni-Vanuatu and Kenyan population by assessing dextromethorphan O-demethylation activity. Drug Metabolism and Pharmacokinetics, 2020, 35, 89-101.	2.2	9
15	Mechanisms of Deamidation of Asparagine Residues and Effects of Main-Chain Conformation on Activation Energy. International Journal of Molecular Sciences, 2020, 21, 7035.	4.1	17
16	Molecular Dynamics Simulations for Three-Dimensional Structures of Orotate Phosphoribosyltransferases Constructed from a Simplified Amino Acid Set. ACS Omega, 2020, 5, 13069-13076.	3.5	5
17	Influence of the conformations of Î±A-crystallin peptides on the isomerization rates of aspartic acid residues. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2020, 1868, 140480.	2.3	2
18	Computational studies on nonenzymatic succinimide-formation mechanisms of the aspartic acid residues catalyzed by two water molecules. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2020, 1868, 140459.	2.3	5

#	Article	IF	Citations
19	Computational studies on nonenzymatic pyroglutamylation mechanism of N-terminal glutamic acid residues in aqueous conditions*. Molecular Physics, 2020, 118, e1702727.	1.7	4
20	Computational Studies on the Mechanisms of Nonenzymatic Intramolecular Cyclization of the Glutamine Residues Located at N-Termini Catalyzed by Inorganic Phosphate Species. ACS Omega, 2020, 5, 9162-9170.	3.5	5
21	Development of Force Field Parameters for <i>p</i>-Carborane to Investigate the Structural Influence of Carborane Derivatives on Drug Targets by Complex Formation. Biological and Pharmaceutical Bulletin, 2020, 43, 1931-1939.	1.4	1
22	Three dimensional structures of putative, primitive proteins to investigate the origin of homochirality. Scientific Reports, 2019, 9, 11594.	3.3	11
23	Computational Studies on Water-Catalyzed Mechanisms for Stereoinversion of Glutarimide Intermediates Formed from Glutamic Acid Residues in Aqueous Phase. International Journal of Molecular Sciences, 2019, 20, 2410.	4.1	2
24	Possible Mechanisms of Nonenzymatic Formation of Dehydroalanine Residue Catalyzed by Dihydrogen Phosphate Ion. Journal of Physical Chemistry B, 2019, 123, 3147-3155.	2.6	12
25	Computational Studies on the Nonenzymatic Deamidation Mechanisms of Glutamine Residues. ACS Omega, 2019, 4, 3508-3513.	3.5	17
26	Computational studies on the waterâ€catalyzed stereoinversion mechanism of glutamic acid residues in peptides and proteins. Chirality, 2018, 30, 527-535.	2.6	5
27	Computational studies on non-succinimide-mediated stereoinversion mechanism of aspartic acid residues assisted by phosphate. Molecular Physics, 2018, 116, 686-696.	1.7	0
28	Influences of conformations of peptides on stereoinversions and/or isomerizations of aspartic acid residues. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2018, 1866, 783-788.	2.3	7
29	Comparison of the activation energy barrier for succinimide formation from Î±- and Î²-aspartic acid residues obtained from density functional theory calculations. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2018, 1866, 759-766.	2.3	16
30	Validation of molecular force field parameters for peptides including isomerized amino acids. Chirality, 2018, 30, 332-341.	2.6	6
31	Theoretical study on ketoâ€“enol tautomerisation of glutarimide for exploration of the isomerisation reaction pathway of glutamic acid in proteins using density functional theory. Molecular Physics, 2017, 115, 560-565.	1.7	7
32	Validation of Molecular Dynamics Simulations for Prediction of Three-Dimensional Structures of Small Proteins. Molecules, 2017, 22, 1716.	3.8	49