Kaori Fukuzawa

List of Publications by Year
in descending order

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Version: 2024-02-01

117	3,876	109137	143772
papers	citations	35 h-index	57 g-index

127	127	127	1988
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Fragment molecular orbital method: use of approximate electrostatic potential. Chemical Physics Letters, 2002, 351, 475-480.	1.2	395
2	Electron-correlated fragment-molecular-orbital calculations for biomolecular and nano systems. Physical Chemistry Chemical Physics, 2014, 16, 10310-10344.	1.3	251
3	Ab initio quantum mechanical study of the binding energies of human estrogen receptor ? with its ligands: An application of fragment molecular orbital method. Journal of Computational Chemistry, 2005, 26, 1-10.	1.5	132
4	The Translation Inhibitor Rocaglamide Targets a Bimolecular Cavity between eIF4A and Polypurine RNA. Molecular Cell, 2019, 73, 738-748.e9.	4.5	128
5	VISCANA:Â Visualized Cluster Analysis of Proteinâ^'Ligand Interaction Based on the ab Initio Fragment Molecular Orbital Method for Virtual Ligand Screening. Journal of Chemical Information and Modeling, 2006, 46, 221-230.	2.5	127
6	Molecular Interactions between Estrogen Receptor and Its Ligand Studied by the ab Initio Fragment Molecular Orbital Method. Journal of Physical Chemistry B, 2006, 110, 16102-16110.	1.2	118
7	Large scale FMO-MP2 calculations on a massively parallel-vector computer. Chemical Physics Letters, 2008, 457, 396-403.	1.2	113
8	Fragment molecular orbital method: application to molecular dynamics simulation, â€˜ab initio FMO-MDâ€™. Chemical Physics Letters, 2003, 372, 342-347.	1.2	112
9	Intra- and intermolecular interactions between cyclic-AMP receptor protein and DNA:Ab initio fragment molecular orbital study. Journal of Computational Chemistry, 2006, 27, 948-960.	1.5	107
10	A configuration analysis for fragment interaction. Chemical Physics Letters, 2005, 410, 247-253.	1.2	87
11	Fragment Molecular Orbital Based Interaction Analyses on COVID-19 Main Protease â^' Inhibitor N3 Complex (PDB ID: 6LU7). Journal of Chemical Information and Modeling, 2020, 60, 3593-3602.	2.5	84
12	Higher-order correlated calculations based on fragment molecular orbital scheme. Theoretical Chemistry Accounts, 2011, 130, 515-530.	0.5	78
13	Selfâ€Degradable Lipidâ€Like Materials Based on â€œHydrolysis accelerated by the intraâ€Particle Enrichment of Reactant (HyPER)â€• for Messenger RNA Delivery. Advanced Functional Materials, 2020, 30, 1910575.	7.8	65
14	Molecular Orbital Study of Neutralâ€Neutral Reactions concerning HC3N Formation in Interstellar Space. Astrophysical Journal, 1997, 489, 113-121.	1.6	57
15	Development of the four-body corrected fragment molecular orbital (FMO4) method. Chemical Physics Letters, 2012, 523, 128-133.	1.2	56
16	A Molecular Orbital Study of the documentclass{aastex} usepackage{amsbsy} usepackage{amsfonts} usepackage{amssymb} usepackage{bm} usepackage{mathrsfs} usepackage{pifont} usepackage{stmaryrd} usepackage{textcomp} usepackage{portland,xspace} usepackage{amsmath,amsxtra} usepackage[OT2,OT1]{fontenc} ewcommandcyr{ enewcommandmdefault{wncyr} enewcommandsfdefault{wncyss} enewcommandencodingdefault{OT2} ormalfont selectfont} DeclareTextFontCommand{extcyr}	1.6	55
17	Fragment molecular orbital calculations on large scale systems containing heavy metal atom. Chemical Physics Letters, 2006, 427, 159-165.	1.2	53
18	Theoretical analysis of binding specificity of influenza viral hemagglutinin to avian and human receptors based on the fragment molecular orbital method. Computational Biology and Chemistry, 2008, 32, 198-211.	1.1	52

#	Article	IF	Citations
19	Possibility of Mutation Prediction of Influenza Hemagglutinin by Combination of Hemadsorption Experiment and Quantum Chemical Calculation for Antibody Binding. Journal of Physical Chemistry B, 2009, 113, 4991-4994.	1.2	49
20	Are Neutralâ€Neutral Reactions Effective for the Carbonâ€Chain Growth of Cyanopolyynes and Polyacetylenes in Interstellar Space?. Astrophysical Journal, 1998, 505, 278-285.	1.6	48
21	Three- and four-body corrected fragment molecular orbital calculations with a novel subdividing fragmentation method applicable to structure-based drug design. Journal of Molecular Graphics and Modelling, 2013, 41, 31-42.	1.3	48
22	Visualization analysis of inter-fragment interaction energies of CRPâ€“cAMPâ€“DNA complex based on the fragment molecular orbital method. Biophysical Chemistry, 2007, 130, 1-9.	1.5	47
23	Ab Initio Fragment Molecular Orbital Study of Molecular Interactions in Liganded Retinoid X Receptor: Specification of Residues Associated with Ligand Inducible Information Transmission. Journal of Physical Chemistry B, 2008, 112, 12081-12094.	1.2	47
24	Fragment Molecular Orbital Calculations with Implicit Solvent Based on the Poissonâ€“Boltzmann Equation: II. Protein and Its Ligand-Binding System Studies. Journal of Physical Chemistry B, 2019, 123, 957-973.	1.2	46
25	Solubility improvement of epalrestat by layered structure formation via cocrystallization. CrystEngComm, 2017, 19, 2614-2622.	1.3	45
26	Large-scale FMO-MP3 calculations on the surface proteins of influenza virus, hemagglutinin (HA) and neuraminidase (NA). Chemical Physics Letters, 2010, 493, 346-352.	1.2	44
27	DNA and Estrogen Receptor Interaction Revealed by Fragment Molecular Orbital Calculations. Journal of Physical Chemistry B, 2007, 111, 9621-9627.	1.2	43
28	Application of the fragment molecular orbital method for determination of atomic charges on polypeptides. II. Towards an improvement of force fields used for classical molecular dynamics simulations. Chemical Physics Letters, 2009, 467, 417-423.	1.2	42
29	Accuracy of fragmentation in ab initio calculations of hydrated sodium cation. Chemical Physics Letters, 2009, 478, 295-300.	1.2	41
30	Theoretical Analysis of Activity Cliffs among Benzofuranone-Class Pim1 Inhibitors Using the Fragment Molecular Orbital Method with Molecular Mechanics Poissonâ€“Boltzmann Surface Area (FMO+MM-PBSA) Approach. Journal of Chemical Information and Modeling, 2017, 57, 2996-3010.	2.5	41
31	Fragment Molecular Orbital Calculations on Red Fluorescent Proteins (DsRed and mFruits). Journal of Physical Chemistry B, 2009, 113, 1153-1161.	1.2	40
32	Discovery of boron-conjugated 4-anilinoquinazoline as a prolonged inhibitor of EGFR tyrosine kinase. Organic and Biomolecular Chemistry, 2009, 7, 4415.	1.5	40
33	Implementation of Pair Interaction Energy DecompositionAnalysis and Its Applications to Protein-Ligand Systems. Journal of Computer Chemistry Japan, 2015, 14, 1-9.	0.0	40
34	Ab Initio Fragment Molecular Orbital Study of Molecular Interactions between Liganded Retinoid X Receptor and Its Coactivator; Part II:â€‰ Influence of Mutations in Transcriptional Activation Function 2 Activating Domain Core on the Molecular Interactions. Journal of Physical Chemistry A, 2008, 112, 1986-1998.	1.1	37
35	Molecular recognition of SARS-CoV-2 spike glycoprotein: quantum chemical hot spot and epitope analyses. Chemical Science, 2021, 12, 4722-4739.	3.7	37
36	Application of the fragment molecular orbital method for determination of atomic charges on polypeptides. Chemical Physics Letters, 2007, 449, 329-335.	1.2	36

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37	Receptorâ€specific scoring functions derived from quantum chemical models improve affinity estimates for inâ€silico drug discovery. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1264-1273.	1.5	36
38	Developments and applications of ABINIT-MP software based on the fragment molecular orbital method. , 2006, , 39-52.		36
39	Fragment Molecular Orbital Calculations with Implicit Solvent Based on the Poissonâ€“Boltzmann Equation: Implementation and DNA Study. Journal of Physical Chemistry B, 2018, 122, 4457-4471.	1.2	35
40	Ab Initio Fragment Molecular Orbital Study of Molecular Interactions between Liganded Retinoid X Receptor and Its Coactivator:Â Roles of Helix 12 in the Coactivator Binding Mechanism. Journal of Physical Chemistry B, 2007, 111, 3525-3533.	1.2	33
41	Modeling of peptideâ€“silica interaction based on four-body corrected fragment molecular orbital (FMO4) calculations. Chemical Physics Letters, 2013, 566, 25-31.	1.2	30
42	Fragment molecular orbital study of the binding energy of ligands to the estrogen receptor. Pure and Applied Chemistry, 2003, 75, 2405-2410.	0.9	29
43	Fragment Molecular Orbital (FMO) and FMO-MO Calculations of DNA: Accuracy Validation of Energy and Interfragment Interaction Energy. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1328-1337.	0.4	26
44	Prediction of probable mutations in influenza virus hemagglutinin protein based on large-scale ab initio fragment molecular orbital calculations. Journal of Molecular Graphics and Modelling, 2011, 30, 110-119.	1.3	26
45	Development of an automated fragment molecular orbital (FMO) calculation protocol toward construction of quantum mechanical calculation database for large biomolecules . Chem-Bio Informatics Journal, 2019, 19, 5-18.	0.1	26
46	Counterpoise-corrected interaction energy analysis based on the fragment molecular orbital scheme. Chemical Physics Letters, 2011, 509, 67-71.	1.2	24
47	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.	2.5	24
48	Charge Clamps of Lysines and Hydrogen Bonds Play Key Roles in the Mechanism to Fix Helix 12 in the Agonist and Antagonist Positions of Estrogen Receptor Î±: Intramolecular Interactions Studied by the Ab Initio Fragment Molecular Orbital Method. Journal of Physical Chemistry B, 2014, 118, 4993-5008.	1.2	23
49	usepackage{amsfonts} usepackage{amssymb} usepackage{bm} usepackage{mathrsfs} usepackage{pifont} usepackage{stmaryrd} usepackage{textcomp} usepackage{portland,xspace} usepackage{amsmath,amsxtra} usepackage[OT2,OT1]{fontenc} ewcommandcyr{ enewcommandmdefault{wncyr} enewcommandsfdefault{wncyss}	1.6	23
50	Application of singular value decomposition to the inter-fragment interaction energy analysis for ligand screening. Computational and Theoretical Chemistry, 2018, 1132, 23-34.	1.1	22
51	Towards good correlation between fragment molecular orbital interaction energies and experimental IC50 for ligand binding: A case study of p38 MAP kinase. Computational and Structural Biotechnology Journal, 2018, 16, 421-434.	1.9	22
52	Intermolecular interaction among Remdesivir, RNA and RNA-dependent RNA polymerase of SARS-CoV-2 analyzed by fragment molecular orbital calculation. Journal of Molecular Graphics and Modelling, 2020, 100, 107695.	1.3	22
53	High-Precision Atomic Charge Prediction for Protein Systems Using Fragment Molecular Orbital Calculation and Machine Learning. Journal of Chemical Information and Modeling, 2020, 60, 3361-3368.	2.5	22
54	Intermolecular Interaction Analyses on SARS-CoV-2 Spike Protein Receptor Binding Domain and Human Angiotensin-Converting Enzyme 2 Receptor-Blocking Antibody/Peptide Using Fragment Molecular Orbital Calculation. Journal of Physical Chemistry Letters, 2021, 12, 4059-4066.	2.1	22

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55	Fragment molecular orbital calculations for biomolecules. Current Opinion in Structural Biology, 2022, 72, 127-134.	2.6	21
56	Explicit solvation modulates intra- and inter-molecular interactions within DNA: Electronic aspects revealed by the ab initio fragment molecular orbital (FMO) method. Computational and Theoretical Chemistry, 2015, 1054, 29-37.	1.1	20
57	Modeling of hydroxyapatiteâ€“peptide interaction based on fragment molecular orbital method. Chemical Physics Letters, 2015, 629, 58-64.	1.2	20
58	Interaction analyses of SARS-CoV-2 spike protein based on fragment molecular orbital calculations. RSC Advances, 2021, 11, 3272-3279.	1.7	20
59	Novel type of virtual ligand screening on the basis of quantum-chemical calculations for proteinâ€“ligand complexes and extended clustering techniques. Computational and Theoretical Chemistry, 2015, 1061, 12-22.	1.1	19
60	Numerical Methodology of Sodium-Water Reaction with Multiphase Flow Analysis. Nuclear Science and Engineering, 2005, 150, 221-236.	0.5	18
61	Fragment molecular orbital (FMO) study on stabilization mechanism of neuro-oncological ventral antigen (NOVA)â€“RNA complex system. Computational and Theoretical Chemistry, 2010, 962, 45-55.	1.5	18
62	Partial geometry optimization with FMO-MP2 gradient: Application to TrpCage. Chemical Physics Letters, 2012, 535, 157-162.	1.2	18
63	Comparison of Epitope Structures of H3HAs through Protein Modeling of Influenza A Virus Hemagglutinin: Mechanism for Selection of Antigenic Variants in the Presence of a Monoclonal Antibody. Microbiology and Immunology, 2007, 51, 1179-1187.	0.7	17
64	Interaction energy analysis on specific binding of influenza virus hemagglutinin to avian and human sialosaccharide receptors: Importance of mutation-induced structural change. Journal of Molecular Graphics and Modelling, 2014, 53, 48-58.	1.3	17
65	Folding simulation of small proteins by dissipative particle dynamics (DPD) with non-empirical interaction parameters based on fragment molecular orbital calculations. Applied Physics Express, 2020, 13, 017002.	1.1	17
66	Dynamic Cooperativity of Ligandâ€“Residue Interactions Evaluated with the Fragment Molecular Orbital Method. Journal of Physical Chemistry B, 2021, 125, 6501-6512.	1.2	17
67	Antigenâ€“antibody interactions of influenza virus hemagglutinin revealed by the fragment molecular orbital calculation. Theoretical Chemistry Accounts, 2011, 130, 1197-1202.	0.5	16
68	Accuracy of the fragment molecular orbital (FMO) calculations for DNA: Total energy, molecular orbital, and inter-fragment interaction energy. Computational and Theoretical Chemistry, 2014, 1034, 7-16.	1.1	16
69	Sialic Acid Recognition of the Pandemic Influenza 2009 H1N1 Virus: Binding Mechanism Between Human Receptor and Influenza Hemagglutinin. Protein and Peptide Letters, 2011, 18, 530-539.	0.4	15
70	Fragment molecular orbital (FMO) calculations on DNA by a scaled third-order MÃ¸ller-Plesset perturbation (MP2.5) scheme. Computational and Theoretical Chemistry, 2017, 1101, 46-54.	1.1	15
71	Identification of correlated inter-residue interactions in protein complex based on the fragment molecular orbital method. Journal of Molecular Graphics and Modelling, 2020, 100, 107650.	1.3	15
72	Molecular action of larvicidal flavonoids on ecdysteroidogenic glutathione S-transferase Noppera-bo in Aedes aegypti. BMC Biology, 2022, 20, 43.	1.7	15

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73	An integrated approach to unravel a crucial structural property required for the function of the insect steroidogenic Halloween protein Noppera-bo. Journal of Biological Chemistry, 2020, 295, 7154-7167.	1.6	14
74	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
75	Hydration of ligands of influenza virus neuraminidase studied by the fragment molecular orbital method. Journal of Molecular Graphics and Modelling, 2016, 69, 144-153.	1.3	12
76	Destabilization of DNA through interstrand crosslinking by UO22+. Chemical Communications, 2019, 55, 2015-2018.	2.2	12
77	Statistical interaction analyses between SARS-CoV-2 main protease and inhibitor N3 by combining molecular dynamics simulation and fragment molecular orbital calculation. Applied Physics Express, 2021, 14, 027003.	1.1	12
78	The ABINIT-MP Program. , 2021, , 53-67.		10
79	Stabilization mechanism of amorphous carbamazepine by transglycosylated rutin, a non-polymeric amorphous additive with a high glass transition temperature. International Journal of Pharmaceutics, 2021, 600, 120491.	2.6	10
80	Special Features of COVID-19 in the FMODB: Fragment Molecular Orbital Calculations and Interaction Energy Analysis of SARS-CoV-2-Related Proteins. Journal of Chemical Information and Modeling, 2021, 61, 4594-4612.	2.5	10
81	Proteinâ€“ligand binding affinity prediction of cyclinâ€dependent kinaseâ€2 inhibitors by dynamically averaged fragment molecular orbitalâ€based interaction energy. Journal of Computational Chemistry, 2022, 43, 1362-1371.	1.5	10
82	An ab initio and experimental study of vibrational effects in low energy O++C2H2 charge-transfer collisions. Journal of Chemical Physics, 2001, 115, 3184-3194.	1.2	9
83	Explicit solvation of a single-stranded DNA, a binding protein,Âand their complex: a suitable protocol forÂfragment molecular orbital calculation. Chem-Bio Informatics Journal, 2017, 17, 72-84.	0.1	8
84	Interaction between a Single-Stranded DNA and a Binding Protein Viewed by the Fragment Molecular Orbital Method. Bulletin of the Chemical Society of Japan, 2018, 91, 1596-1605.	2.0	7
85	Effect of sulfobutyl ether-Î²-cyclodextrin and propylene glycol alginate on the solubility of clozapine. Pharmaceutical Development and Technology, 2019, 24, 479-486.	1.1	7
86	How to Perform FMO Calculation in Drug Discovery. , 2021, , 93-125.		7
87	Taking Water into Account with the Fragment Molecular Orbital Method. Methods in Molecular Biology, 2020, 2114, 105-122.	0.4	7
88	Collective residue interactions in trimer complexes of SARS-CoV-2 spike proteins analyzed by fragment molecular orbital method. Applied Physics Express, 2022, 15, 017001.	1.1	7
89	Formation Mechanism of Lipid Membrane and Vesicle Using Small Angle X-ray Scattering and Dissipative Particle Dynamics (DPD) Method. Journal of Computer Chemistry Japan, 2018, 17, 172-179.	0.0	6
90	Interaction between calcite and adsorptive peptide analyzed by fragment molecular orbital method. Japanese Journal of Applied Physics, 2019, 58, 120906.	0.8	6

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91	Ab initio potential energy surfaces of the ion-molecule reaction: C2H2+O+. Journal of Chemical Physics, 2004, 121, 3117-3129.	1.2	4
92	A Preliminary Study of Correction for Inter Fragment Interaction Energy (IFIE) between Fragments Sharing Bond Detached Atom (BDA). Journal of Computer Aided Chemistry, 2017, 18, 143-148.	0.3	4
93	Machine learning prediction of inter-fragment interaction energies between ligand and amino-acid residues on the fragment molecular orbital calculations for Janus kinase â€“ inhibitor complex. Chemical Physics Letters, 2020, 757, 137883.	1.2	4
94	Fragmentation at sp 2 carbon atoms in fragment molecular orbital method. Journal of Computational Chemistry, 2020, 41, 1416-1420.	1.5	4
95	Computational Ab Initio Interaction Analyses between Neutralizing Antibody and SARS-CoV-2 Variant Spike Proteins Using the Fragment Molecular Orbital Method. Bulletin of the Chemical Society of Japan, 2021, 94, 1794-1798.	2.0	4
96	Epalrestat tetrahydrofuran monosolvate: crystal structure and phase transition. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 941-944.	0.2	3
97	Manufacturability and Properties of Granules and Tablets Using the Eco-Friendly Granulation Method Green Fluidized Bed Granulation Compared to Direct Compression. Chemical and Pharmaceutical Bulletin, 2021, 69, 447-455.	0.6	3
98	Development Status of ABINIT-MP in 2020. Journal of Computer Chemistry Japan, 2020, 19, 142-145.	0.0	3
99	The GTP responsiveness of PI5P4Kî² evolved from a compromised trade-off between activity and specificity. Structure, 2022, 30, 886-899.e4.	1.6	3
100	Evaluating the correlation of binding affinities between isothermal titration calorimetry and fragment molecular orbital method of estrogen receptor beta with diarylpropionitrile (DPN) or DPN derivatives. Journal of Steroid Biochemistry and Molecular Biology, 2022, 222, 106152.	1.2	3
101	Crystal Structural Analysis of DL-Mandelate Salt of Carvedilol and Its Correlation with Physicochemical Properties. Crystals, 2020, 10, 53.	1.0	2
102	Crystal Structure of Novel Terephthalate Salt of Antiarrhythmic Drug Disopyramide. Crystals, 2021, 11, 368.	1.0	2
103	Altered Media Flow and Tablet Position as Factors of How Air Bubbles Affect Dissolution of Disintegrating and Non-disintegrating Tablets Using a USP 4 Flow-Through Cell Apparatus. AAPS PharmSciTech, 2021, 22, 227.	1.5	2
104	A new solvate of epalerstat, a drug for diabetic neuropathy. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 1264-1267.	0.2	2
105	Computational approach to elucidate the formation and stabilization mechanism of amorphous formulation using molecular dynamics simulation and fragment molecular orbital calculation. International Journal of Pharmaceutics, 2022, 615, 121477.	2.6	2
106	Sulfated Hyaluronan Binds to Heparanase and Blocks Its Enzymatic and Cellular Actions in Carcinoma Cells. International Journal of Molecular Sciences, 2022, 23, 5055.	1.8	2
107	Water-mediated interactions in the CRPâ€“cAMPâ€“DNA complex: Does water mediate sequence-specific binding at the DNA primary-kink site?. Computational Biology and Chemistry, 2008, 32, 149-158.	1.1	1
108	Acceleration of Environmental Electrostatic Potential Using Cholesky Decomposition with Adaptive Metric (CDAM) for Fragment Molecular Orbital (FMO) Method. Bulletin of the Chemical Society of Japan, 2021, 94, 91-96.	2.0	1

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109	Crystal Structures of Antiarrhythmic Drug Disopyramide and Its Salt with Phthalic Acid. Crystals, 2021, 11, 379.	1.0	1
110	FMO Drug Design Consortium. , 2021, , 127-181.		1
111	Interaction Analyses between Calcite/Apatite and Peptides by Fragment Molecular Orbital Method. Journal of Computer Chemistry Japan, 2020, 19, 1-7.	0.0	1
112	Accuracy of Dimer-ES Approximation on Fragment Molecular Orbital (FMO) Method . Chem-Bio Informatics Journal, 2018, 18, 119-122.	0.1	0
113	Estimation of Graph Convolutional Network in Ames Prediction of Drug Candidate Compounds. Journal of Computer Chemistry Japan, 2021, 20, 1-9.	0.0	0
114	Modeling of Solid and Surface. , 2021, , 407-424.		0
115	Effects of Water Molecules and Configurations of Neighboring Amino Acid Residues Surrounding DsRed Chromophore on Its Excitation Energy. Journal of Computer Chemistry Japan, 2015, 14, 155-163.	0.0	0
116	Improving the Accuracy of Crystal Structure Prediction Using FMO Crystal Energy: An Example of Target XXIII. Journal of Computer Chemistry Japan, 2021, 20, 92-93.	0.0	0
117	FMO calculations for zinc metalloprotease:Fragmentation of amino-acid residues coordinated to zinc ion. Chem-Bio Informatics Journal, 2022, 22, 21-25.	0.1	0