Qing-Chuan Zheng

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8607211/publications.pdf

Version: 2024-02-01

114 papers	1,056 citations	516710 16 h-index	610901 24 g-index
114 all docs	114 docs citations	114 times ranked	1403 citing authors

#	Article	IF	Citations
1	VARIDT 2.0: structural variability of drug transporter. Nucleic Acids Research, 2022, 50, D1417-D1431.	14.5	65
2	Structural and Dynamic Basis of Human Cytochrome P450â€‰7B1: A Survey of Substrate Selectivity and Major Active Site Access Channels. Chemistry - A European Journal, 2013, 19, 549-557.	3.3	39
3	Molecular Dynamic Investigations of the Mutational Effects on Structural Characteristics and Tunnel Geometry in CYP17A1. Journal of Chemical Information and Modeling, 2013, 53, 3308-3317.	5.4	37
4	A molecular dynamics investigation into the mechanisms of alectinib resistance of three ALK mutants. Journal of Cellular Biochemistry, 2018, 119, 5332-5342.	2.6	33
5	Rational design and synthesis of yellow-light emitting triazole fluorophores with AIE and mechanochromic properties. Chemical Communications, 2019, 55, 4603-4606.	4.1	30
6	Molecular Dynamics Simulations Suggest Ligandâ€™s Binding to Nicotinamidase/Pyrazinamidase. PLoS ONE, 2012, 7, e39546.	2.5	28
7	Fosfomycin Protects Mice From Staphylococcus aureus Pneumonia Caused by Î±-Hemolysin in Extracellular Vesicles by Inhibiting MAPK-Regulated NLRP3 Inflammasomes. Frontiers in Cellular and Infection Microbiology, 2019, 9, 253.	3.9	25
8	Theoretical insights into the reductive metabolism of CCl₄ by cytochrome P450 enzymes and the CCl₄-dependent suicidal inactivation of P450. Dalton Transactions, 2014, 43, 14833-14840.	3.3	24
9	Theoretical studies of the spectroscopic properties of blue emitting iridium complexes. Theoretical Chemistry Accounts, 2008, 121, 155-164.	1.4	22
10	A comparative analysis of binding sites between mouse CYP2C38 and CYP2C39 based on homology modeling, molecular dynamics simulation and docking studies. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2009, 1794, 1066-1072.	2.3	22
11	Influence of Hyperthermophilic Protein Cren7 on the Stability and Conformation of DNA: Insights from Molecular Dynamics Simulation and Free Energy Analysis. Journal of Physical Chemistry B, 2012, 116, 12415-12425.	2.6	22
12	Exploring the Molecular Basis of dsRNA Recognition by Mss116p Using Molecular Dynamics Simulations and Free-Energy Calculations. Langmuir, 2013, 29, 11135-11144.	3.5	21
13	Structural features and dynamic investigations of the membrane-bound cytochrome P450 17A1. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 2013-2021.	2.6	20
14	Revealing the binding and drug resistance mechanism of amprenavir, indinavir, ritonavir, and nelfinavir complexed with HIV-1 protease due to double mutations G48T/L89M by molecular dynamics simulations and free energy analyses. Physical Chemistry Chemical Physics, 2020, 22, 4464-4480.	2.8	20
15	Investigation of ligand selectivity in CYP3A7 by molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2360-2367.	3.5	19
16	Molecular basis of the recognition of arachidonic acid by cytochrome P450 2E1 along major access tunnel. Biopolymers, 2015, 103, 53-66.	2.4	18
17	Heparin makes differences: a molecular dynamics simulation study on the human Î²II-tryptase monomer. Molecular BioSystems, 2015, 11, 252-261.	2.9	17
18	Detoxification of 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP) by cytochrome P450 enzymes: A theoretical investigation. Journal of Inorganic Biochemistry, 2016, 154, 21-28.	3.5	17

#	Article	IF	Citations
19	MD Simulation Investigation on the Binding Process of Smoke-Derived Germination Stimulants to Its Receptor. Journal of Chemical Information and Modeling, 2019, 59, 1554-1562.	5.4	17
20	Exploring the interactional details between aldose reductase (AKR1B1) and 3-Mercapto-5H-1,2,4-triazino[5,6-b]indole-5-acetic acid through molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1724-1735.	3.5	17
21	Molecular dynamics simulations studies and free energy analysis on inhibitors of MDM2â€“p53 interaction. Journal of Molecular Graphics and Modelling, 2013, 46, 132-139.	2.4	16
22	Insights into the effects of mutations on Cren7â€“DNA binding using molecular dynamics simulations and free energy calculations. Physical Chemistry Chemical Physics, 2015, 17, 5704-5711.	2.8	16
23	What are the effects of the serine triad on proton conduction of an influenza B M2 channel? An investigation by molecular dynamics simulations. Physical Chemistry Chemical Physics, 2019, 21, 8820-8826.	2.8	15
24	Multiple Molecular Dynamics Simulations of the Inhibitor GRL-02031 Complex with Wild Type and Mutant HIV-1 Protease Reveal the Binding and Drug-Resistance Mechanism. Langmuir, 2020, 36, 13817-13832.	3.5	15
25	Molecular dynamics investigation on the Asciminib resistance mechanism of I502L and V468F mutations in BCR-ABL. Journal of Molecular Graphics and Modelling, 2019, 89, 242-249.	2.4	14
26	Analysis of clinically relevant substrates of CYP2B6 enzyme by computational methods. Journal of Molecular Modeling, 2011, 17, 2839-2846.	1.8	13
27	Exploring the mechanism how Marburg virus VP35 recognizes and binds dsRNA by molecular dynamics simulations and free energy calculations. Biopolymers, 2014, 101, 849-860.	2.4	13
28	Molecular Dynamics Investigations of Binding Mechanism for Triazoles Inhibitors to CYP51. Frontiers in Molecular Biosciences, 2020, 7, 586540.	3.5	13
29	Homology modeling and substrate binding study of Nudix hydrolase Ndx1 from Thermos thermophilus HB8. Biochemical and Biophysical Research Communications, 2005, 333, 881-887.	2.1	12
30	Insight into the Dynamic Interaction of Different Carbohydrates with Human Surfactant Protein D: Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 7383-7390.	2.6	12
31	Highlighting a Ï€â€“Ï€ interaction: a protein modeling and molecular dynamics simulation study on Anopheles gambiae glutathione S-transferase 1-2. Journal of Molecular Modeling, 2013, 19, 5213-5223.	1.8	12
32	How Does (E)-2-(Acetamidomethylene)succinate Bind to Its Hydrolase? From the Binding Process to the Final Result. PLoS ONE, 2013, 8, e53811.	2.5	12
33	Humanization of fibroblast growth factor 1 singleâ€chain antibody and validation for its antitumorigenic efficacy in breast cancer and glioma cells. Journal of Cellular and Molecular Medicine, 2018, 22, 3259-3263.	3.6	12
34	Exploring the interaction between human focal adhesion kinase and inhibitors: a molecular dynamic simulation and free energy calculations. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2351-2366.	3.5	11
35	Conformational Transition of Key Structural Features Involved in Activation of ALK Induced by Two Neuroblastoma Mutations and ATP Binding: Insight from Accelerated Molecular Dynamics Simulations. ACS Chemical Neuroscience, 2018, 9, 1783-1792.	3.5	11
36	Exploring the interactions of EGFR with phosphorylated Mig6 by molecular dynamics simulations and MM-PBSA calculations. Journal of Theoretical Biology, 2018, 447, 118-125.	1.7	11

#	Article	IF	Citations
37	In Silico Study of Membrane Lipid Composition Regulating Conformation and Hydration of Influenza Virus B M2 Channel. Journal of Chemical Information and Modeling, 2020, 60, 3603-3615.	5.4	11
38	How do mutations affect the structural characteristics and substrate binding of CYP21A2? An investigation by molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 8870-8877.	2.8	11
39	Drug Design Benefits from Molecular Dynamics: Some Examples. Current Computer-Aided Drug Design, 2013, 9, 532-546.	1.2	11
40	Constant pH molecular dynamics (CpHMD) and molecular docking studies of CquiOBP1 pH-induced ligand releasing mechanism. Journal of Molecular Modeling, 2013, 19, 1301-1309.	1.8	10
41	Insights into the epimerization activities of RaCE and pAGE: the quantum mechanics/molecular mechanics simulations. RSC Advances, 2015, 5, 102284-102293.	3.6	10
42	A unique activationâ€“promotion mechanism of the influenza B M2 proton channel uncovered by multiscale simulations. Physical Chemistry Chemical Physics, 2019, 21, 2984-2991.	2.8	9
43	Constant pH Molecular Dynamics (CpHMD) and mutation studies: Insights into AaegOBP1 pH-induced ligand releasing mechanism. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2012, 1824, 913-918.	2.3	8
44	Construction of giant branched nanotubes from cyclodextrin-based supramolecular amphiphiles. Chemical Communications, 2015, 51, 6512-6514.	4.1	8
45	QM/MM calculations and MD simulations of acetolactate decarboxylase to reveal substrate R/S-acetolactate binding mode and stereoselective catalytic mechansim. RSC Advances, 2016, 6, 91852-91859.	3.6	8
46	A strategy of designing the ligand of antibody affinity chromatography based on molecular dynamics simulation. Journal of Chromatography A, 2016, 1463, 81-89.	3.7	8
47	Probing the interaction mechanism of small molecule inhibitors with matriptase based on molecular dynamics simulation and free energy calculations. Journal of Biomolecular Structure and Dynamics, 2017, 35, 755-764.	3.5	8
48	What regulates the catalytic activities in AGE catalysis? An answer from quantum mechanics/molecular mechanics simulations. Physical Chemistry Chemical Physics, 2017, 19, 31731-31746.	2.8	8
49	Optimization of a MT1-MMP-targeting Peptide and Its Application in Near-infrared Fluorescence Tumor Imaging. Scientific Reports, 2018, 8, 10334.	3.3	8
50	Mutation and low pH effect on the stability as well as unfolding kinetics of transthyretin dimer. Biophysical Chemistry, 2014, 189, 8-15.	2.8	7
51	Exploring the structure characteristics and major channels of cytochrome P450 2A6, 2A13, and 2E1 with pilocarpine. Biopolymers, 2018, 109, e23108.	2.4	7
52	In Silico Analysis Revealed a Unique Binding but Ineffective Mode of Amantadine to Influenza Virus B M2 Channel. Journal of Physical Chemistry Letters, 2021, 12, 1169-1174.	4.6	7
53	Multiple Molecular Dynamics Simulations and Free-Energy Predictions Uncover the Susceptibility of Variants of HIV-1 Protease against Inhibitors Darunavir and KNI-1657. Langmuir, 2021, 37, 14407-14418.	3.5	7
54	Homology modelling and molecular dynamics study of human fatty acid amide hydrolase. Molecular Simulation, 2009, 35, 1201-1208.	2.0	6

#	Article	IF	Citations
55	Quantum chemical modeling of 1,1â€proton transfer reaction catalyzed by a cofactorâ€independent Î±â€methylacylâ€CoA racemase. International Journal of Quantum Chemistry, 2012, 112, 619-624.	2.0	6
56	How mutations affecting the ligand-receptor interactions: a combined MD and QM/MM calculation on CYP2E1 and its two mutants. Chemical Research in Chinese Universities, 2015, 31, 1029-1038.	2.6	6
57	Molecular dynamics investigations of BioH protein substrate specificity for biotin synthesis. Journal of Biomolecular Structure and Dynamics, 2016, 34, 1052-1060.	3.5	6
58	Exploring the inhibition mechanism on HIFâ€2 by inhibitor PT2399 and 0X3 using molecular dynamics simulations. Journal of Molecular Recognition, 2018, 31, e2730.	2.1	6
59	Insights into the drug resistance induced by the BaDHPS mutations: molecular dynamic simulations and MM/GBSA studies. Journal of Biomolecular Structure and Dynamics, 2013, 31, 1127-1136.	3.5	5
60	Molecular dynamics (MD) simulations and binding free energy calculation studies between inhibitors and type II dehydroquinase (DHQ2). Molecular Simulation, 2013, 39, 137-144.	2.0	5
61	Insights into the phosphatase and the synthase activities of human bisphosphoglycerate mutase: a quantum mechanics/molecular mechanics simulation. Physical Chemistry Chemical Physics, 2014, 16, 3946.	2.8	5
62	Exploring the mechanism how AF9 recognizes and binds H3K9ac by molecular dynamics simulations and free energy calculations. Biopolymers, 2016, 105, 779-786.	2.4	5
63	Effect of External Electric Field on Substrate Transport of a Secondary Active Transporter. Journal of Chemical Information and Modeling, 2016, 56, 1539-1546.	5.4	5
64	Theoretical research in structure characteristics of different inhibitors and differences of binding modes with CBP bromodomain. Bioorganic and Medicinal Chemistry, 2018, 26, 712-720.	3.0	5
65	Exploring the allosteric mechanism of protein tyrosine phosphatase 1B by molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4040-4047.	3.5	5
66	Exploring the Allosteric Mechanism of Src Homology-2 Domain-Containing Protein Tyrosine Phosphatase 2 (SHP2) by Molecular Dynamics Simulations. Frontiers in Chemistry, 2020, 8, 597495.	3.6	5
67	What are the effects of cucurbit[n]uril on CTMS loading? Insights from QM calculations and MD simulations. Computational Materials Science, 2020, 181, 109751.	3.0	5
68	A novel benzotriazole derivate with Twisted intramolecular charge transfer and Aggregation Induced emission features for proton determination. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 269, 120780.	3.9	5
69	Investigation of the molecular and mechanistic basis for the regioselective metabolism of midazolam by cytochrome P450 3A4. Physical Chemistry Chemical Physics, 2022, 24, 8104-8112.	2.8	5
70	Evaluating substrate specificity of glutathione peroxidase mimic by molecular dynamics simulations and kinetics. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2008, 60, 139-144.	1.6	4
71	HOMOLOGY MODELING AND SUBSTRATE BINDING STUDY OF HUMAN KYNURENINE AMINOTRANSFERASE III. Journal of Theoretical and Computational Chemistry, 2012, 11, 855-870.	1.8	4
72	Insights into the thermal stabilization and conformational transitions of DNA by hyperthermophile protein Sso7d: molecular dynamics simulations and MM-PBSA analysis. Journal of Biomolecular Structure and Dynamics, 2012, 30, 716-727.	3.5	4

#	Article	IF	Citations
73	A molecular dynamics and computational study of human KAT3 involved in KYN pathway. Science China Chemistry, 2013, 56, 514-523.	8.2	4
74	Natural velvet antler polypeptide conformation prediction and molecular docking study with TGF-Î²1 complex. Journal of Molecular Modeling, 2013, 19, 3671-3682.	1.8	4
75	Bio-activation of 4-alkyl analogs of 1,4-dihydropyridine mediated by cytochrome P450 enzymes. Journal of Biological Inorganic Chemistry, 2015, 20, 665-673.	2.6	4
76	2D-QSAR study, molecular docking, and molecular dynamics simulation studies of interaction mechanism between inhibitors and transforming growth factor-beta receptor I (ALK5). Journal of Biomolecular Structure and Dynamics, 2018, 36, 3705-3717.	3.5	4
77	Molecular dynamics investigation of stereoselective inhibition mechanism of HIFâ€2Î±/ARNT heterodimer. Journal of Molecular Recognition, 2018, 31, e2675.	2.1	4
78	Insight on mutationâ€induced resistance to anaplastic lymphoma kinase inhibitor ceritinib from molecular dynamics simulations. Biopolymers, 2019, 110, e23257.	2.4	4
79	Multiple Molecular Dynamics Simulations and Energy Analysis Unravel the Dynamic Properties and Binding Mechanism of Mutants HIV-1 Protease with DRV and CA-p2. Microbiology Spectrum, 2022, , e0074821.	3.0	4
80	Theoretical studies of interaction models of human acetylcholine esterase with different inhibitors. Science in China Series B: Chemistry, 2009, 52, 1911-1916.	0.8	3
81	Molecular dynamic studies on Langmuir monolayers of stearic acid. Chemical Research in Chinese Universities, 2013, 29, 545-550.	2.6	3
82	Molecular simulation investigation on the interaction between barrier-to-autointegration factor or its Gly25Glu mutant and DNA. Journal of Molecular Modeling, 2014, 20, 2246.	1.8	3
83	Fosfomycin Induced Structural Change in Fosfomycin Resistance Kinases FomA: Molecular Dynamics and Molecular Docking Studies. Journal of Molecular Modeling, 2014, 20, 2236.	1.8	3
84	Exploring the influence of hyperthermophilic protein Ssh10b on the stability and conformation of RNA by molecular dynamics simulation. Biopolymers, 2018, 109, e23068.	2.4	3
85	How Chorismatases Regulate Distinct Reaction Channels in a Single Conserved Active Pocket: Mechanistic Analysis with QM/MM (ONIOM) Investigations. Chemistry - A European Journal, 2019, 25, 1326-1336.	3.3	3
86	Key Factors in Conformation Transformation of an Important Neuronic Protein Glucose Transport 3 Revealed by Molecular Dynamics Simulation. ACS Chemical Neuroscience, 2019, 10, 4444-4448.	3.5	3
87	Molecular dynamics simulations study of influence of Tyr422Ala mutation on transcriptional enhancer activation domain 4 (TEAD4) and transcription co-activators complexes. Journal of Theoretical Biology, 2019, 472, 27-35.	1.7	3
88	Purified Vitexin Compound 1 Inhibits UVA-Induced Cellular Senescence in Human Dermal Fibroblasts by Binding Mitogen-Activated Protein Kinase 1. Frontiers in Cell and Developmental Biology, 2020, 8, 691.	3.7	3
89	Exploring the Distinct Binding and Activation Mechanisms for Different CagA Oncoproteins and SHP2 by Molecular Dynamics Simulations. Molecules, 2021, 26, 837.	3.8	3
90	Theoretical investigations on the effects of mutations in important residues of NS1B on its RNA-binding using molecular dynamics simulations. Computers in Biology and Medicine, 2022, 145, 105412.	7.0	3

#	Article	IF	Citations
91	Homology modeling and PAPS ligand (cofactor) binding study of bovine phenol sulfotransferase. Journal of Molecular Modeling, 2005, 11, 97-104.	1.8	2
92	Influence of C-terminal tail deletion on structure and stability of hyperthermophile Sulfolobus tokodaii RNase HI. Journal of Molecular Modeling, 2013, 19, 2647-2656.	1.8	2
93	Theoretical investigation on binding process of allophanate to allophanate hydrolase. Chemical Research in Chinese Universities, 2015, 31, 1023-1028.	2.6	2
94	Molecular basis of the recognition of FMN by a HAD phosphatase TON_0338. Journal of Molecular Graphics and Modelling, 2016, 69, 17-25.	2.4	2
95	Exploring the mechanism of how tvMyb2 recognizes and binds ap65-1 by molecular dynamics simulations and free energy calculations. Molecular BioSystems, 2016, 12, 76-84.	2.9	2
96	Studying the recognition mechanism of TcaR and ssDNA using molecular dynamic simulations. Journal of Molecular Graphics and Modelling, 2018, 80, 67-75.	2.4	2
97	Recognition mechanism of Wilmsâ€™ tumour suppressor protein and DNA triplets: insights from molecular dynamics simulation and free energy analysis. Journal of Biomolecular Structure and Dynamics, 2019, 37, 562-575.	3.5	2
98	A theoretical study on the signal transduction process of bacterial photoreceptor PpSB1 based on the Markov state model. Physical Chemistry Chemical Physics, 2021, 23, 2398-2405.	2.8	2
99	Studies of Interaction Mechanism between Pyrido [3,4-d] Pyrimidine Inhibitors and Mps1. Molecules, 2021, 26, 5075.	3.8	2
100	The regioselectivity of the interaction between dextromethorphan and CYP2D6. Physical Chemistry Chemical Physics, 2022, 24, 2234-2242.	2.8	2
101	Molecular Basis of the Recognition of Cholesterol by Cytochrome P450 46A1 along the Major Access Tunnel. ACS Chemical Neuroscience, 2022, , .	3.5	2
102	A quantum mechanics study on the reaction mechanism of chalcone formation from p-coumaroyl-CoA and malonyl-CoA catalyzed by chalcone synthase. Theoretical Chemistry Accounts, 2009, 122, 157-166.	1.4	1
103	Theoretical study on the mechanism of rearrangement reaction catalyzed by N5-carboxyaminoimidazole ribonucleotide mutase. Computational and Theoretical Chemistry, 2011, 964, 77-82.	2.5	1
104	Computational modelling of novel inhibitors targeting the human GSTP1*D homology domain. Molecular Simulation, 2013, 39, 550-562.	2.0	1
105	Insight into the urea binding and K166R mutation stabilizing mechanism of TlpB: Molecular dynamics and principal component analysis study. Chemical Research in Chinese Universities, 2014, 30, 1011-1017.	2.6	1
106	Theoretical evaluation and improvement on the potency of the rhodanine-based inhibitors for human serotoninN-acetyltransferase. Molecular Simulation, 2014, 40, 1201-1208.	2.0	1
107	Molecular simulation investigation on the interaction between barrier-to-autointegration factor dimer or its Gly25Glu mutant and LEM domain of emerin. Computational Biology and Chemistry, 2014, 53, 184-190.	2.3	1
108	A selective and sensitive fluorescence probe for Se(IV) based on fluorescence quenching of gatifloxacin. Chemical Research in Chinese Universities, 2016, 32, 736-741.	2.6	1

#	Article	IF	Citations
109	Predicting a Kind of Unusual Multiple-States Dimerization-Modes Transformation in Protein PD-L1 System by Computational Investigation and a Generalized Rate Theory. Frontiers in Chemistry, 2021, 9, 783444.	3.6	1
110	How DNA affects the hyperthermophilic protein Ape10b2 for oligomerization: an investigation using multiple short molecular dynamics simulations. Physical Chemistry Chemical Physics, 2021, 23, 25841-25849.	2.8	1
111	Conformational Changes of Enzymes and DNA in Molecular Dynamics. Advances in Protein Chemistry and Structural Biology, 2013, 92, 179-217.	2.3	0
112	The influence of residue in the position of 116 on the inhibitory potency of TH588 for MTH1. Journal of Molecular Graphics and Modelling, 2018, 85, 75-83.	2.4	0
113	Exploring three important drug resistance mutations in ALK with three different inhibitors: insight from molecular simulations. Panminerva Medica, 2021, , .	0.8	0
114	A molecular dynamics investigation into the mechanisms of tvMyb2 recognizes and binds ap65-1. Minerva Surgery, 2024, 79, .	0.6	0