# Qing-Chuan Zheng

List of Publications by Year
in descending order

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|---|---|---|---|
| 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 | A molecular dynamics investigation into the mechanisms of tvMyb2 recognizes and binds ap65-1. Minerva Surgery, 2024, 79, . | 0.6 | 0 |
| 2 | VARIDT 2.0: structural variability of drug transporter. Nucleic Acids Research, 2022, 50, D1417-D1431. | 14.5 | 65 |
| 3 | 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 |
| 4 | The regioselectivity of the interaction between dextromethorphan and CYP2D6. Physical Chemistry Chemical Physics, 2022, 24, 2234-2242. | 2.8 | 2 |
| 5 | 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 |
| 6 | 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 |
| 7 | 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 |
| 8 | Molecular Basis of the Recognition of Cholesterol by Cytochrome P450 46A1 along the Major Access Tunnel. ACS Chemical Neuroscience, 2022, , . | 3.5 | 2 |
| 9 | 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 |
| 10 | 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 |
| 11 | Exploring the Distinct Binding and Activation Mechanisms for Different CagA Oncoproteins and SHP2 by Molecular Dynamics Simulations. Molecules, 2021, 26, 837. | 3.8 | 3 |
| 12 | Exploring three important drug resistance mutations in ALK with three different inhibitors: insight from molecular simulations. Panminerva Medica, 2021, , . | 0.8 | 0 |
| 13 | Studies of Interaction Mechanism between Pyrido [3,4-d] Pyrimidine Inhibitors and Mps1. Molecules, 2021, 26, 5075. | 3.8 | 2 |
| 14 | 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 |
| 15 | 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 |
| 16 | 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 |
| 17 | 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 |
| 18 | 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 |

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| 19 | 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 |
| 20 | 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 |
| 21 | 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 |
| 22 | 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 |
| 23 | 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 |
| 24 | 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 |
| 25 | Molecular Dynamics Investigations of Binding Mechanism for Triazoles Inhibitors to CYP51. Frontiers in Molecular Biosciences, 2020, 7, 586540. | 3.5 | 13 |
| 26 | 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 |
| 27 | 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 |
| 28 | 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 |
| 29 | 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 |
| 30 | 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 |
| 31 | Rational design and synthesis of yellow-light emitting triazole fluorophores with AIE and mechanochromic properties. Chemical Communications, 2019, 55, 4603-4606. | 4.1 | 30 |
| 32 | 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 |
| 33 | Insight on mutationâ€induced resistance to anaplastic lymphoma kinase inhibitor ceritinib from molecular dynamics simulations. Biopolymers, 2019, 110, e23257. | 2.4 | 4 |
| 34 | 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 |
| 35 | 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 |
| 36 | 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 |

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| 37 | 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 |
| 38 | Exploring the structure characteristics and major channels of cytochrome P450 2A6, 2A13, and 2E1 with pilocarpine. Biopolymers, 2018, 109, e23108. | 2.4 | 7 |
| 39 | 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 |
| 40 | 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 |
| 41 | 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 |
| 42 | 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 |
| 43 | 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 |
| 44 | 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 |
| 45 | 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 |
| 46 | Molecular dynamics investigation of stereoselective inhibition mechanism of HIFâ€2Î±/ARNT heterodimer. Journal of Molecular Recognition, 2018, 31, e2675. | 2.1 | 4 |
| 47 | 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 |
| 48 | 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 |
| 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 | 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 |
| 51 | 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 |
| 52 | 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 |
| 53 | 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 |
| 54 | 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 |

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| 55 | 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 |
| 56 | 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 |
| 57 | 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 |
| 58 | 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 |
| 59 | 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 |
| 60 | 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 |
| 61 | 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 |
| 62 | Molecular dynamics investigations of BioH protein substrate specificity for biotin synthesis. Journal of Biomolecular Structure and Dynamics, 2016, 34, 1052-1060. | 3.5 | 6 |
| 63 | Structural features and dynamic investigations of the membrane-bound cytochrome P450 17A1. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 2013-2021. | 2.6 | 20 |
| 64 | 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 |
| 65 | Theoretical investigation on binding process of allophanate to allophanate hydrolase. Chemical Research in Chinese Universities, 2015, 31, 1023-1028. | 2.6 | 2 |
| 66 | Heparin makes differences: a molecular dynamics simulation study on the human Î²II-tryptase monomer. Molecular BioSystems, 2015, 11, 252-261. | 2.9 | 17 |
| 67 | 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 |
| 68 | Investigation of ligand selectivity in CYP3A7 by molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2360-2367. | 3.5 | 19 |
| 69 | 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 |
| 70 | Construction of giant branched nanotubes from cyclodextrin-based supramolecular amphiphiles. Chemical Communications, 2015, 51, 6512-6514. | 4.1 | 8 |
| 71 | Insights into the epimerization activities of RaCE and pAGE: the quantum mechanics/molecular mechanics simulations. RSC Advances, 2015, 5, 102284-102293. | 3.6 | 10 |
| 72 | Molecular basis of the recognition of arachidonic acid by cytochrome P450 2E1 along major access tunnel. Biopolymers, 2015, 103, 53-66. | 2.4 | 18 |

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| 73 | 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 |
| 74 | 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 |
| 75 | 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 |
| 76 | 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 |
| 77 | 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 |
| 78 | Theoretical insights into the reductive metabolism of CCl<sub>4</sub> by cytochrome P450 enzymes and the CCl<sub>4</sub>-dependent suicidal inactivation of P450. Dalton Transactions, 2014, 43, 14833-14840. | 3.3 | 24 |
| 79 | 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 |
| 80 | 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 |
| 81 | 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 |
| 82 | A molecular dynamics and computational study of human KAT3 involved in KYN pathway. Science China Chemistry, 2013, 56, 514-523. | 8.2 | 4 |
| 83 | Molecular dynamic studies on Langmuir monolayers of stearic acid. Chemical Research in Chinese Universities, 2013, 29, 545-550. | 2.6 | 3 |
| 84 | 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 |
| 85 | 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 |
| 86 | 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 |
| 87 | 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 |
| 88 | Conformational Changes of Enzymes and DNA in Molecular Dynamics. Advances in Protein Chemistry and Structural Biology, 2013, 92, 179-217. | 2.3 | 0 |
| 89 | 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 |
| 90 | 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 |

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| 91 | 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 |
| 92 | 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 |
| 93 | 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 |
| 94 | Computational modelling of novel inhibitors targeting the human GSTP1*D homology domain. Molecular Simulation, 2013, 39, 550-562. | 2.0 | 1 |
| 95 | 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 |
| 96 | 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 |
| 97 | Drug Design Benefits from Molecular Dynamics: Some Examples. Current Computer-Aided Drug Design, 2013, 9, 532-546. | 1.2 | 11 |
| 98 | 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 |
| 99 | HOMOLOGY MODELING AND SUBSTRATE BINDING STUDY OF HUMAN KYNURENINE AMINOTRANSFERASE III. Journal of Theoretical and Computational Chemistry, 2012, 11, 855-870. | 1.8 | 4 |
| 100 | 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 |
| 101 | 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 |
| 102 | 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 |
| 103 | Molecular Dynamics Simulations Suggest Ligandâ€™s Binding to Nicotinamidase/Pyrazinamidase. PLoS ONE, 2012, 7, e39546. | 2.5 | 28 |
| 104 | Analysis of clinically relevant substrates of CYP2B6 enzyme by computational methods. Journal of Molecular Modeling, 2011, 17, 2839-2846. | 1.8 | 13 |
| 105 | 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 |
| 106 | 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 |
| 107 | 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 |
| 108 | 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 |

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| 109 | 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 |
| 110 | Homology modelling and molecular dynamics study of human fatty acid amide hydrolase. Molecular Simulation, 2009, 35, 1201-1208. | 2.0 | 6 |
| 111 | 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 |
| 112 | Theoretical studies of the spectroscopic properties of blue emitting iridium complexes. Theoretical Chemistry Accounts, 2008, 121, 155-164. | 1.4 | 22 |
| 113 | Homology modeling and PAPS ligand (cofactor) binding study of bovine phenol sulfotransferase. Journal of Molecular Modeling, 2005, 11, 97-104. | 1.8 | 2 |
| 114 | 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 |