Yajun Zheng

List of Publications by Year
in descending order

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48 papers	2,519 citations	257450 24 h-index	214800 47 g-index
49 all docs	49 docs citations	49 times ranked	3204 citing authors

#	Article	IF	Citations
1	Insights into Proteinâ€“Ligand Interactions in Integrin Complexes: Advances in Structure Determinations. Journal of Medicinal Chemistry, 2020, 63, 5675-5696.	6.4	23
2	Discovery of Potent Inhibitors of 11Î²-Hydroxysteroid Dehydrogenase Type 1 Using a Novel Growth-Based Protocol of in Silico Screening and Optimization in CONTOUR. Journal of Chemical Information and Modeling, 2019, 59, 3422-3436.	5.4	5
3	Conformational control in structure-based drug design. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 2825-2837.	2.2	38
4	The utilization of spirocyclic scaffolds in novel drug discovery. Expert Opinion on Drug Discovery, 2016, 11, 831-834.	5.0	179
5	Non-canonical modulators of nuclear receptors. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 4157-4164.	2.2	24
6	Brain penetrant liver X receptor (LXR) modulators based on a 2,4,5,6-tetrahydropyrrolo[3,4-c]pyrazole core. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 5044-5050.	2.2	10
7	Discovery of a Novel, Orally Efficacious Liver X Receptor (LXR) Î² Agonist. Journal of Medicinal Chemistry, 2016, 59, 3264-3271.	6.4	29
8	Identification of spirooxindole and dibenzoxazepine motifs as potent mineralocorticoid receptor antagonists. Bioorganic and Medicinal Chemistry, 2016, 24, 1384-1391.	3.0	24
9	The use of spirocyclic scaffolds in drug discovery. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 3673-3682.	2.2	739
10	Structure-Based Design of Î²-Site APP Cleaving Enzyme 1 (BACE1) Inhibitors for the Treatment of Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2013, 56, 4156-4180.	6.4	126
11	Recent Advances in Mineralocorticoid Receptor Antagonists. Annual Reports in Medicinal Chemistry, 2011, , 89-102.	0.9	4
12	Computational Characterization of Metal Binding Groups for Metalloenzyme Inhibitors. Journal of Chemical Theory and Computation, 2006, 2, 990-996.	5.3	3
13	Conformational flexibility of antifungal atropisomeric strobilurin analogues: a quantum mechanical investigation. Computational and Theoretical Chemistry, 2005, 719, 69-74.	1.5	6
14	A Novel Class of Inhibitors of Peptide Deformylase Discovered through High-Throughput Screening and Virtual Ligand Screening. Journal of Medicinal Chemistry, 2004, 47, 6669-6672.	6.4	50
15	Quinoprotein methanol dehydrogenase: a molecular dynamics study and comparison with crystal structure. Journal of Molecular Structure, 2003, 655, 269-277.	3.6	10
16	Examination of a reaction intermediate in the active site of riboflavin synthase. Bioorganic Chemistry, 2003, 31, 278-287.	4.1	3
17	Reaction of 2,2-Bis(trifluoromethyl)-1,1-dicyanoethylene with 6,6-Dimethylfulvene:Â Cycloadditions and a Rearrangement. Journal of Organic Chemistry, 2003, 68, 120-129.	3.2	14
18	Protein Engineering of Nitrile Hydratase Activity of Papain:Â Molecular Dynamics Study of a Mutant and Wild-Type Enzyme. Journal of the American Chemical Society, 2002, 124, 12979-12990.	13.7	14

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19	Inhibition of Fungal Aldose Reductase. Protein and Peptide Letters, 2001, 8, 407-412.	0.9	1
20	Synthesis and structural analysis of the active enantiomer of famoxadone, a potent inhibitor of cytochrome bc 1. Bioorganic and Medicinal Chemistry Letters, 2000, 10, 1059-1062.	2.2	13
21	Solvolytic Enolization of Scytalone. Organic Letters, 2000, 2, 1541-1544.	4.6	6
22	The Structures of the Enzymeâ€“Substrate Complex and Transition State Formed in the SN2 Displacement of Clâ¯from 1,2-Dichloroethane at the Active Site ofXanthobacter autotrophicusHaloalkane Dehalogenase. Bioorganic Chemistry, 1998, 26, 169-174.	4.1	2
23	Rapid Enzyme-Catalyzed Heterolytic Câ¯H Bond Cleavage by a Base Strength Amplification Mechanism:Â A Theoretical Examination of the Mechanism of Oxidation of Vitamin K. Journal of the American Chemical Society, 1998, 120, 1623-1624.	13.7	6
24	Theoretical Investigation of the Hydride Transfer from Formate to NAD+and the Implications for the Catalytic Mechanism of Formate Dehydrogenase. Journal of the American Chemical Society, 1998, 120, 7192-7200.	13.7	32
25	Molecular Dynamics Simulations of Ground and Transition States for the SN2 Displacement of Cl- from 1,2-Dichloroethane at the Active Site of Xanthobacter autotrophicus Haloalkane Dehalogenase. Journal of the American Chemical Society, 1998, 120, 5611-5621.	13.7	59
26	Role of a critical water in scytalone dehydratase-catalyzed reaction. Proceedings of the National Academy of Sciences of the United States of America, 1998, 95, 4158-4163.	7.1	16
27	Nonenzymatic and enzymatic hydrolysis of alkyl halides: A theoretical study of the SN2 reactions of acetate and hydroxide ions with alkyl chlorides. Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 6591-6595.	7.1	31
28	Conformation of coenzyme pyrroloquinoline quinone and role of Ca2+ in the catalytic mechanism of quinoprotein methanol dehydrogenase. Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 11881-11886.	7.1	59
29	A Theoretical Examination of the Factors Controlling the Catalytic Efficiency of a Transmethylation Enzyme:Â CatecholO-Methyltransferase. Journal of the American Chemical Society, 1997, 119, 8137-8145.	13.7	81
30	Role of Active Site Tyrosine in Glutathione S-Transferase:â€‰ Insights from a Theoretical Study on Model Systems. Journal of the American Chemical Society, 1997, 119, 1523-1528.	13.7	31
31	Ab Initio Quantum Mechanics Analysis of Imidazole C-Hâ€¦O Water Hydrogen Bonding and a Molecular Mechanics Forcefield Correction. Journal of Biomolecular Structure and Dynamics, 1997, 14, 657-665.	3.5	34
32	On the Dehalogenation Mechanism of 4-Chlorobenzoyl CoA by 4-Chlorobenzoyl CoA Dehalogenase:Â Insights from Study Based on the Nonenzymatic Reaction. Journal of the American Chemical Society, 1997, 119, 3868-3877.	13.7	33
33	Non-enzymatic and enzymatic hydrolysis of alkyl halides: A haloalkane dehalogenation enzyme evolved to stabilize the gas-phase transition state of an SN2 displacement reaction. Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 8417-8420.	7.1	53
34	Is strong hydrogen bonding in the transition state enough to account for the observed rate acceleration in a mutant of papain?. Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 4285-4288.	7.1	14
35	A density functional theory investigation of metal ion binding sites in monosaccharides. Computational and Theoretical Chemistry, 1997, 389, 233-240.	1.5	29
36	Identifying the Intermediate in the Dioxygen Transfer from 4a-Hydroperoxyflavin Anion to Phenolate and Indole Anions. Bioorganic Chemistry, 1997, 25, 331-336.	4.1	4

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37	A Theoretical Study of the Structures of Flavin in Different Oxidation and Protonation States. Journal of the American Chemical Society, 1996, 118, 9402-9408.	13.7	120
38	What Happens to Salt-Bridges in Nonaqueous Environments:Â Insights from Quantum Mechanics Calculations. Journal of the American Chemical Society, 1996, 118, 11237-11243.	13.7	60
39	A Molecular Dynamics and Quantum Mechanics Analysis of the Effect of DMSO on Enzyme Structure and Dynamics:Â Subtilisin. Journal of the American Chemical Society, 1996, 118, 4175-4180.	13.7	102
40	Molecular dynamics of subtilisin Carlsberg in aqueous and nonaqueous solutions. , 1996, 38, 791-799.		13
41	Catalytic Role of the Î±-Carboxylate of the Glu Residue of Glutathione in Glutathione S-transferases. Journal of Biomolecular Structure and Dynamics, 1996, 14, 231-233.	3.5	1
42	An explanation of the single-turnover experiment of 4-chlorobenzoyl CoA dehalogenase. Protein Engineering, Design and Selection, 1996, 9, 721-723.	2.1	6
43	A force field for monosaccharides and (1 ? 4) linked polysaccharides. Journal of Computational Chemistry, 1994, 15, 1019-1040.	3.3	121
44	Theoretical examination of the mechanism of aldoseâ€“ketose isomerization. Protein Engineering, Design and Selection, 1993, 6, 479-484.	2.1	31
45	Mechanism of the human carbonic anhydrase II-catalyzed hydration of carbon dioxide. Journal of the American Chemical Society, 1992, 114, 10498-10507.	13.7	108
46	Conformational preferences for hydroxyl groups in substituted tetrahydropyrans. Journal of Computational Chemistry, 1992, 13, 772-791.	3.3	36
47	Study of hydrogen bonding interactions relevant to biomolecular structure and function. Journal of Computational Chemistry, 1992, 13, 1151-1169.	3.3	114
48	A theoretical study of the HP4 ion. Inorganic Chemistry, 1991, 30, 3361-3362.	4.0	2