

# 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	The use of spirocyclic scaffolds in drug discovery. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2014, 24, 3673-3682.	2.2	739
2	The utilization of spirocyclic scaffolds in novel drug discovery. <i>Expert Opinion on Drug Discovery</i> , 2016, 11, 831-834.	5.0	179
3	Structure-Based Design of Î²-Site APP Cleaving Enzyme 1 (BACE1) Inhibitors for the Treatment of Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 4156-4180.	6.4	126
4	A force field for monosaccharides and (1 ? 4) linked polysaccharides. <i>Journal of Computational Chemistry</i> , 1994, 15, 1019-1040.	3.3	121
5	A Theoretical Study of the Structures of Flavin in Different Oxidation and Protonation States. <i>Journal of the American Chemical Society</i> , 1996, 118, 9402-9408.	13.7	120
6	Study of hydrogen bonding interactions relevant to biomolecular structure and function. <i>Journal of Computational Chemistry</i> , 1992, 13, 1151-1169.	3.3	114
7	Mechanism of the human carbonic anhydrase II-catalyzed hydration of carbon dioxide. <i>Journal of the American Chemical Society</i> , 1992, 114, 10498-10507.	13.7	108
8	A Molecular Dynamics and Quantum Mechanics Analysis of the Effect of DMSO on Enzyme Structure and Dynamics: A Subtilisin. <i>Journal of the American Chemical Society</i> , 1996, 118, 4175-4180.	13.7	102
9	A Theoretical Examination of the Factors Controlling the Catalytic Efficiency of a Transmethylation Enzyme: A Catechol O-Methyltransferase. <i>Journal of the American Chemical Society</i> , 1997, 119, 8137-8145.	13.7	81
10	What Happens to Salt-Bridges in Nonaqueous Environments: A Insights from Quantum Mechanics Calculations. <i>Journal of the American Chemical Society</i> , 1996, 118, 11237-11243.	13.7	60
11	Conformation of coenzyme pyrroloquinoline quinone and role of Ca <sup>2+</sup> in the catalytic mechanism of quinoprotein methanol dehydrogenase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1997, 94, 11881-11886.	7.1	59
12	Molecular Dynamics Simulations of Ground and Transition States for the SN <sub>2</sub> Displacement of Cl <sup>-</sup> from 1,2-Dichloroethane at the Active Site of <i>Xanthobacter autotrophicus</i> Haloalkane Dehalogenase. <i>Journal of the American Chemical Society</i> , 1998, 120, 5611-5621.	13.7	59
13	Non-enzymatic and enzymatic hydrolysis of alkyl halides: A haloalkane dehalogenation enzyme evolved to stabilize the gas-phase transition state of an SN <sub>2</sub> displacement reaction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1997, 94, 8417-8420.	7.1	53
14	A Novel Class of Inhibitors of Peptide Deformylase Discovered through High-Throughput Screening and Virtual Ligand Screening. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 6669-6672.	6.4	50
15	Conformational control in structure-based drug design. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2017, 27, 2825-2837.	2.2	38
16	Conformational preferences for hydroxyl groups in substituted tetrahydropyrans. <i>Journal of Computational Chemistry</i> , 1992, 13, 772-791.	3.3	36
17	Ab Initio Quantum Mechanics Analysis of Imidazole C-H...O Water Hydrogen Bonding and a Molecular Mechanics Forcefield Correction. <i>Journal of Biomolecular Structure and Dynamics</i> , 1997, 14, 657-665.	3.5	34
18	On the Dehalogenation Mechanism of 4-Chlorobenzoyl CoA by 4-Chlorobenzoyl CoA Dehalogenase: A Insights from Study Based on the Nonenzymatic Reaction. <i>Journal of the American Chemical Society</i> , 1997, 119, 3868-3877.	13.7	33

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19	Theoretical Investigation of the Hydride Transfer from Formate to NAD <sup>+</sup> and the Implications for the Catalytic Mechanism of Formate Dehydrogenase. <i>Journal of the American Chemical Society</i> , 1998, 120, 7192-7200.	13.7	32
20	Theoretical examination of the mechanism of aldose↔ketose isomerization. <i>Protein Engineering, Design and Selection</i> , 1993, 6, 479-484.	2.1	31
21	Nonenzymatic and enzymatic hydrolysis of alkyl halides: A theoretical study of the SN <sub>2</sub> reactions of acetate and hydroxide ions with alkyl chlorides. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1997, 94, 6591-6595.	7.1	31
22	Role of Active Site Tyrosine in Glutathione S-Transferase: Insights from a Theoretical Study on Model Systems. <i>Journal of the American Chemical Society</i> , 1997, 119, 1523-1528.	13.7	31
23	A density functional theory investigation of metal ion binding sites in monosaccharides. <i>Computational and Theoretical Chemistry</i> , 1997, 389, 233-240.	1.5	29
24	Discovery of a Novel, Orally Efficacious Liver X Receptor (LXR) $\hat{1}^2$ Agonist. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 3264-3271.	6.4	29
25	Non-canonical modulators of nuclear receptors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2016, 26, 4157-4164.	2.2	24
26	Identification of spirooxindole and dibenzoxazepine motifs as potent mineralocorticoid receptor antagonists. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 1384-1391.	3.0	24
27	Insights into Protein↔Ligand Interactions in Integrin Complexes: Advances in Structure Determinations. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 5675-5696.	6.4	23
28	Role of a critical water in scytalone dehydratase-catalyzed reaction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1998, 95, 4158-4163.	7.1	16
29	Is strong hydrogen bonding in the transition state enough to account for the observed rate acceleration in a mutant of papain?. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1997, 94, 4285-4288.	7.1	14
30	Protein Engineering of Nitrile Hydratase Activity of Papain: A Molecular Dynamics Study of a Mutant and Wild-Type Enzyme. <i>Journal of the American Chemical Society</i> , 2002, 124, 12979-12990.	13.7	14
31	Reaction of 2,2-Bis(trifluoromethyl)-1,1-dicyanoethylene with 6,6-Dimethylfulvene: Cycloadditions and a Rearrangement. <i>Journal of Organic Chemistry</i> , 2003, 68, 120-129.	3.2	14
32	Molecular dynamics of subtilisin Carlsberg in aqueous and nonaqueous solutions. , 1996, 38, 791-799.		13
33	Synthesis and structural analysis of the active enantiomer of famoxadone, a potent inhibitor of cytochrome bc 1. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2000, 10, 1059-1062.	2.2	13
34	Quinoprotein methanol dehydrogenase: a molecular dynamics study and comparison with crystal structure. <i>Journal of Molecular Structure</i> , 2003, 655, 269-277.	3.6	10
35	Brain penetrant liver X receptor (LXR) modulators based on a 2,4,5,6-tetrahydropyrrolo[3,4-c]pyrazole core. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2016, 26, 5044-5050.	2.2	10
36	An explanation of the single-turnover experiment of 4-chlorobenzoyl CoA dehalogenase. <i>Protein Engineering, Design and Selection</i> , 1996, 9, 721-723.	2.1	6

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37	Rapid Enzyme-Catalyzed Heterolytic C-H Bond Cleavage by a Base Strength Amplification Mechanism: A Theoretical Examination of the Mechanism of Oxidation of Vitamin K. <i>Journal of the American Chemical Society</i> , 1998, 120, 1623-1624.	13.7	6
38	Solvolytic Enolization of Scytalone. <i>Organic Letters</i> , 2000, 2, 1541-1544.	4.6	6
39	Conformational flexibility of antifungal atropisomeric strobilurin analogues: a quantum mechanical investigation. <i>Computational and Theoretical Chemistry</i> , 2005, 719, 69-74.	1.5	6
40	Discovery of Potent Inhibitors of 11 $\beta$ -Hydroxysteroid Dehydrogenase Type 1 Using a Novel Growth-Based Protocol of <i>in Silico</i> Screening and Optimization in CONTOUR. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3422-3436.	5.4	5
41	Identifying the Intermediate in the Dioxygen Transfer from 4a-Hydroperoxyflavin Anion to Phenolate and Indole Anions. <i>Bioorganic Chemistry</i> , 1997, 25, 331-336.	4.1	4
42	Recent Advances in Mineralocorticoid Receptor Antagonists. <i>Annual Reports in Medicinal Chemistry</i> , 2011, , 89-102.	0.9	4
43	Examination of a reaction intermediate in the active site of riboflavin synthase. <i>Bioorganic Chemistry</i> , 2003, 31, 278-287.	4.1	3
44	Computational Characterization of Metal Binding Groups for Metalloenzyme Inhibitors. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 990-996.	5.3	3
45	A theoretical study of the HP4 ion. <i>Inorganic Chemistry</i> , 1991, 30, 3361-3362.	4.0	2
46	The Structures of the Enzyme-Substrate Complex and Transition State Formed in the SN2 Displacement of Cl <sup>-</sup> from 1,2-Dichloroethane at the Active Site of <i>Xanthobacter autotrophicus</i> Haloalkane Dehalogenase. <i>Bioorganic Chemistry</i> , 1998, 26, 169-174.	4.1	2
47	Catalytic Role of the $\hat{\pm}$ -Carboxylate of the Glu Residue of Glutathione in Glutathione S-transferases. <i>Journal of Biomolecular Structure and Dynamics</i> , 1996, 14, 231-233.	3.5	1
48	Inhibition of Fungal Aldose Reductase. <i>Protein and Peptide Letters</i> , 2001, 8, 407-412.	0.9	1