Chang-Guo Zhan

List of Publications by Year
in descending order

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289 papers	10,905 citations	34016 52 h-index	48187 88 g-index

295 all docs	295 docs citations	295 times ranked	10114 citing authors

#	Article	IF	Citations
1	Ionization Potential, Electron Affinity, Electronegativity, Hardness, and Electron Excitation Energy:â€‰Molecular Properties from Density Functional Theory Orbital Energies. Journal of Physical Chemistry A, 2003, 107, 4184-4195.	1.1	1,134
2	A novel Hsp90 inhibitor to disrupt Hsp90/Cdc37 complex against pancreatic cancer cells. Molecular Cancer Therapeutics, 2008, 7, 162-170.	1.9	338
3	The Tumor Inhibitor and Antiangiogenic Agent Withaferin A Targets the Intermediate Filament Protein Vimentin. Chemistry and Biology, 2007, 14, 623-634.	6.2	283
4	Absolute Hydration Free Energy of the Proton from First-Principles Electronic Structure Calculations. Journal of Physical Chemistry A, 2001, 105, 11534-11540.	1.1	277
5	Identify potent SARS-CoV-2 main protease inhibitors via accelerated free energy perturbation-based virtual screening of existing drugs. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 27381-27387.	3.3	174
6	Computational redesign of human butyrylcholinesterase for anticocaine medication. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 16656-16661.	3.3	171
7	Hydration of the Fluoride Anion:Â Structures and Absolute Hydration Free Energy from First-Principles Electronic Structure Calculations. Journal of Physical Chemistry A, 2004, 108, 2020-2029.	1.1	166
8	Most Efficient Cocaine Hydrolase Designed by Virtual Screening of Transition States. Journal of the American Chemical Society, 2008, 130, 12148-12155.	6.6	164
9	Electron Affinities of AlnClusters and Multiple-Fold Aromaticity of the Square Al42-Structure. Journal of the American Chemical Society, 2002, 124, 14795-14803.	6.6	162
10	Volume polarization in reaction field theory. Journal of Chemical Physics, 1998, 108, 177-192.	1.2	132
11	Fundamental Reaction Mechanism for Cocaine Hydrolysis in Human Butyrylcholinesterase. Journal of the American Chemical Society, 2003, 125, 2462-2474.	6.6	131
12	Subnanomolar Inhibitor of Cytochrome bc₁ Complex Designed by Optimizing Interaction with Conformationally Flexible Residues. Journal of the American Chemical Society, 2010, 132, 185-194.	6.6	110
13	Catalytic Mechanism of Cytochrome P450 for 5â€²-Hydroxylation of Nicotine: Fundamental Reaction Pathways and Stereoselectivity. Journal of the American Chemical Society, 2011, 133, 7416-7427.	6.6	110
14	Reaction Pathways and Energy Barriers for Alkaline Hydrolysis of Carboxylic Acid Esters in Water Studied by a Hybrid Supermolecule-Polarizable Continuum Approach. Journal of the American Chemical Society, 2000, 122, 2621-2627.	6.6	107
15	The Nature and Absolute Hydration Free Energy of the Solvated Electron in Water. Journal of Physical Chemistry B, 2003, 107, 4403-4417.	1.2	107
16	Cavity size in reaction field theory. Journal of Chemical Physics, 1998, 109, 10543-10558.	1.2	105
17	First-Principles Determination of the Absolute Hydration Free Energy of the Hydroxide Ionâ€. Journal of Physical Chemistry A, 2002, 106, 9737-9744.	1.1	105
18	Fundamental Reaction Pathway and Free Energy Profile for Inhibition of Proteasome by Epoxomicin. Journal of the American Chemical Society, 2012, 134, 10436-10450.	6.6	100

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19	Modeling the Catalysis of Anti-Cocaine Catalytic Antibody: Competing Reaction Pathways and Free Energy Barriers. Journal of the American Chemical Society, 2008, 130, 5140-5149.	6.6	97
20	Reaction field effects on nitrogen shielding. Journal of Chemical Physics, 1999, 110, 1611-1622.	1.2	86
21	Determination of Two Structural Forms of Catalytic Bridging Ligand in Zincâ^'Phosphotriesterase by Molecular Dynamics Simulation and Quantum Chemical Calculation. Journal of the American Chemical Society, 1999, 121, 7279-7282.	6.6	83
22	Ligand-Based Virtual Screening Approach Using a New Scoring Function. Journal of Chemical Information and Modeling, 2012, 52, 963-974.	2.5	83
23	Decomposition Pathways of Peroxynitrous Acid:â€‰ Gas-Phase and Solution Energetics. Journal of Physical Chemistry A, 2002, 106, 3191-3196.	1.1	81
24	Thermostable Variants of Cocaine Esterase for Long-Time Protection against Cocaine Toxicity. Molecular Pharmacology, 2009, 75, 318-323.	1.0	81
25	Design, Preparation, and Characterization of High-Activity Mutants of Human Butyrylcholinesterase Specific for Detoxification of Cocaine. Molecular Pharmacology, 2011, 79, 290-297.	1.0	81
26	How Dopamine Transporter Interacts with Dopamine: Insights from Molecular Modeling and Simulation. Biophysical Journal, 2007, 93, 3627-3639.	0.2	79
27	Combined 3D-QSAR Modeling and Molecular Docking Study on Indolinone Derivatives as Inhibitors of 3-Phosphoinositide-Dependent Protein Kinase-1. Journal of Chemical Information and Modeling, 2008, 48, 1760-1772.	2.5	76
28	Free Energy Perturbation (FEP) Simulation on the Transition States of Cocaine Hydrolysis Catalyzed by Human Butyrylcholinesterase and Its Mutants. Journal of the American Chemical Society, 2007, 129, 13537-13543.	6.6	74
29	Mobility of the Active Site Bound Paraoxon and Sarin in Zinc-Phosphotriesterase by Molecular Dynamics Simulation and Quantum Chemical Calculation. Journal of the American Chemical Society, 2001, 123, 817-826.	6.6	72
30	Molecular Dynamics Simulation of Cocaine Binding with Human Butyrylcholinesterase and Its Mutants. Journal of Physical Chemistry B, 2005, 109, 4776-4782.	1.2	72
31	Mechanism for Cocaine Blocking the Transport of Dopamine: Insights from Molecular Modeling and Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 15057-15066.	1.2	72
32	First-Principles Calculation of pK_a for Cocaine, Nicotine, Neurotransmitters, and Anilines in Aqueous Solution. Journal of Physical Chemistry B, 2007, 111, 10599-10605.	1.2	71
33	Catalytic Mechanisms for Cofactor-Free Oxidase-Catalyzed Reactions: Reaction Pathways of Uricase-Catalyzed Oxidation and Hydration of Uric Acid. ACS Catalysis, 2017, 7, 4623-4636.	5.5	71
34	Energy Barriers for Alkaline Hydrolysis of Carboxylic Acid Esters in Aqueous Solution by Reaction Field Calculations. Journal of Physical Chemistry A, 2000, 104, 7672-7678.	1.1	70
35	First Computational Evidence for a Catalytic Bridging Hydroxide Ion in a Phosphodiesterase Active Site. Journal of the American Chemical Society, 2001, 123, 2835-2838.	6.6	69
36	Computational Design of a Human Butyrylcholinesterase Mutant for Accelerating Cocaine Hydrolysis Based on the Transition-State Simulation. Angewandte Chemie - International Edition, 2006, 45, 653-657.	7.2	69

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37	Molecular insights into the mechanism of 4â€hydroxyphenylpyruvate dioxygenase inhibition: enzyme kinetics, Xâ€ray crystallography and computational simulations. FEBS Journal, 2019, 286, 975-990.	2.2	68
38	A highly efficient cocaine-detoxifying enzyme obtained by computational design. Nature Communications, 2014, 5, 3457.	5.8	67
39	Catalytic Mechanism and Energy Barriers for Butyrylcholinesterase-Catalyzed Hydrolysis of Cocaine. Biophysical Journal, 2005, 89, 3863-3872.	0.2	65
40	Characterization of a high-activity mutant of human butyrylcholinesterase against (â^')-cocaine. Chemico-Biological Interactions, 2010, 187, 148-152.	1.7	62
41	Crystal Structure of 4-Hydroxyphenylpyruvate Dioxygenase in Complex with Substrate Reveals a New Starting Point for Herbicide Discovery. Research, 2019, 2019, 2602414.	2.8	62
42	How Can (â^')-Epigallocatechin Gallate from Green Tea Prevent HIV-1 Infection? Mechanistic Insights from Computational Modeling and the Implication for Rational Design of Anti-HIV-1 Entry Inhibitors. Journal of Physical Chemistry B, 2006, 110, 2910-2917.	1.2	61
43	Structure-based methods for predicting target mutation-induced drug resistance and rational drug design to overcome the problem. Drug Discovery Today, 2012, 17, 1121-1126.	3.2	60
44	Uricases as Therapeutic Agents to Treat Refractory Gout: Current States and Future Directions. Drug Development Research, 2012, 73, 66-72.	1.4	59
45	Reaction Pathway and Free Energy Profile for Papain-Catalyzed Hydrolysis of N-Acetyl-Phe-Gly 4-Nitroanilide. Biochemistry, 2013, 52, 5145-5154.	1.2	59
46	Theoretical Studies of Fundamental Pathways for Alkaline Hydrolysis of Carboxylic Acid Esters in Gas Phase. Journal of the American Chemical Society, 2000, 122, 1522-1530.	6.6	58
47	Free-Energy Perturbation Simulation on Transition States and Redesign of Butyrylcholinesterase. Biophysical Journal, 2009, 96, 1931-1938.	0.2	58
48	Theoretical Studies of the Transition-State Structures and Free Energy Barriers for Base-Catalyzed Hydrolysis of Amides. Journal of Physical Chemistry A, 2006, 110, 12644-12652.	1.1	56
49	Long-acting cocaine hydrolase for addiction therapy. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 422-427.	3.3	56
50	Coordination number of zinc ions in the phosphotriesterase active site by molecular dynamics and quantum mechanics. Journal of Computational Chemistry, 2003, 24, 368-378.	1.5	54
51	Assessing the Regioselectivity of OleD-Catalyzed Glycosylation with a Diverse Set of Acceptors. Journal of Natural Products, 2013, 76, 279-286.	1.5	54
52	Arylquins target vimentin to trigger Par-4 secretion for tumor cell apoptosis. Nature Chemical Biology, 2014, 10, 924-926.	3.9	54
53	QSAR modeling of mono- and bis-quaternary ammonium salts that act as antagonists at neuronal nicotinic acetylcholine receptors mediating dopamine release. Bioorganic and Medicinal Chemistry, 2006, 14, 3017-3037.	1.4	53
54	Reaction Pathway and Free-Energy Barrier for Reactivation of Dimethylphosphoryl-Inhibited Human Acetylcholinesterase. Journal of Physical Chemistry B, 2009, 113, 16226-16236.	1.2	53

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55	Fundamental Reaction Mechanism and Free Energy Profile for (â^')-Cocaine Hydrolysis Catalyzed by Cocaine Esterase. Journal of the American Chemical Society, 2009, 131, 11964-11975.	6.6	53
56	Free Energies of Solvation with Surface, Volume, and Local Electrostatic Effects and Atomic Surface Tensions to Represent the First Solvation Shell. Journal of Chemical Theory and Computation, 2010, 6, 1109-1117.	2.3	53
57	Accurate heats of formation and acidities for H3PO4, H2SO4, and H2CO3 from ab initio electronic structure calculations. International Journal of Quantum Chemistry, 2005, 102, 775-784.	1.0	52
58	Modeling Effects of Oxyanion Hole on the Ester Hydrolysis Catalyzed by Human Cholinesterases. Journal of Physical Chemistry B, 2005, 109, 23070-23076.	1.2	52
59	Active Site Gating and Substrate Specificity of Butyrylcholinesterase and Acetylcholinesterase: Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 8797-8805.	1.2	52
60	Are pharmacokinetic approaches feasible for treatment of cocaine addiction and overdose?. Future Medicinal Chemistry, 2012, 4, 125-128.	1.1	52
61	First-principle studies of intermolecular and intramolecular catalysis of protonated cocaine. Journal of Computational Chemistry, 2005, 26, 980-986.	1.5	50
62	Modeling evolution of hydrogen bonding and stabilization of transition states in the process of cocaine hydrolysis catalyzed by human butyrylcholinesterase. Proteins: Structure, Function and Bioinformatics, 2005, 62, 99-110.	1.5	50
63	Fluorinated N,N-Dialkylaminostilbenes Repress Colon Cancer by Targeting Methionine S-Adenosyltransferase 2A. ACS Chemical Biology, 2013, 8, 796-803.	1.6	50
64	Improved Prediction of Bloodâ€“Brain Barrier Permeability Through Machine Learning with Combined Use of Molecular Property-Based Descriptors and Fingerprints. AAPS Journal, 2018, 20, 54.	2.2	50
65	Computational Design and Discovery of Conformationally Flexible Inhibitors of Acetohydroxyacid Synthase to Overcome Drug Resistance Associated with the W586L Mutation. ChemMedChem, 2008, 3, 1203-1206.	1.6	49
66	Understanding the Mechanism of Drug Resistance Due to a Codon Deletion in Protoporphyrinogen Oxidase through Computational Modeling. Journal of Physical Chemistry B, 2009, 113, 4865-4875.	1.2	47
67	Reaction Pathway and Free Energy Profile for Butyrylcholinesterase-Catalyzed Hydrolysis of Acetylcholine. Journal of Physical Chemistry B, 2011, 115, 1315-1322.	1.2	47
68	Novel human mPGES-1 inhibitors identified through structure-based virtual screening. Bioorganic and Medicinal Chemistry, 2011, 19, 6077-6086.	1.4	47
69	Mutation of Tyrosine 470 of Human Dopamine Transporter is Critical for HIV-1 Tat-Induced Inhibition of Dopamine Transport and Transporter Conformational Transitions. Journal of NeuroImmune Pharmacology, 2013, 8, 975-987.	2.1	47
70	Absolute Binding Free Energy Calculation and Design of a Subnanomolar Inhibitor of Phosphodiesterase-10. Journal of Medicinal Chemistry, 2019, 62, 2099-2111.	2.9	47
71	Modeling Multiple Species of Nicotine and Deschloroepibatidine Interacting with Î±4Î²2 Nicotinic Acetylcholine Receptor:Â From Microscopic Binding to Phenomenological Binding Affinity. Journal of the American Chemical Society, 2005, 127, 14401-14414.	6.6	46
72	Modeling Subtype-Selective Agonists Binding with Î±4Î²2 and Î±7 Nicotinic Acetylcholine Receptors:Â Effects of Local Binding and Long-Range Electrostatic Interactions. Journal of Medicinal Chemistry, 2006, 49, 7661-7674.	2.9	46

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73	Structure-and-mechanism-based design and discovery of therapeutics for cocaine overdose and addiction. Organic and Biomolecular Chemistry, 2008, 6, 836-843.	1.5	46
74	Theoretical Studies of Competing Reaction Pathways and Energy Barriers for Alkaline Ester Hydrolysis of Cocaine. Journal of Physical Chemistry A, 2001, 105, 1296-1301.	1.1	45
75	Theoretical Determination of Two Structural Forms of the Active Site in Cadmium-Containing Phosphotriesterases. Journal of Physical Chemistry B, 2002, 106, 717-722.	1.2	45
76	Structural analysis of thermostabilizing mutations of cocaine esterase. Protein Engineering, Design and Selection, 2010, 23, 537-547.	1.0	45
77	Understanding Microscopic Binding of Human Microsomal Prostaglandin E Synthase-1 (mPGES-1) Trimer with Substrate PGH₂ and Cofactor GSH: Insights from Computational Alanine Scanning and Site-directed Mutagenesis. Journal of Physical Chemistry B, 2010, 114, 5605-5616.	1.2	45
78	Computational Mutation Scanning and Drug Resistance Mechanisms of HIV-1 Protease Inhibitors. Journal of Physical Chemistry B, 2010, 114, 9663-9676.	1.2	45
79	Proteasome Inhibitors with Pyrazole Scaffolds from Structure-Based Virtual Screening. Journal of Medicinal Chemistry, 2015, 58, 2036-2041.	2.9	45
80	Design of High-Activity Mutants of Human Butyrylcholinesterase against (â˜)-Cocaine: Structural and Energetic Factors Affecting the Catalytic Efficiency. Biochemistry, 2010, 49, 9113-9119.	1.2	44
81	Modeling of Pharmacokinetics of Cocaine in Human Reveals the Feasibility for Development of Enzyme Therapies for Drugs of Abuse. PLoS Computational Biology, 2012, 8, e1002610.	1.5	43
82	Computational Simulations of the Interactions between Acetyl-Coenzyme-A Carboxylase and Clodinafop: Resistance Mechanism Due to Active and Nonactive Site Mutations. Journal of Chemical Information and Modeling, 2009, 49, 1936-1943.	2.5	42
83	Model of Human Butyrylcholinesterase Tetramer by Homology Modeling and Dynamics Simulation. Journal of Physical Chemistry B, 2009, 113, 6543-6552.	1.2	42
84	Understanding the structureâ€“activity and structureâ€“selectivity correlation of cyclic guanine derivatives as phosphodiesterase-5 inhibitors by molecular docking, CoMFA and CoMSIA analyses. Bioorganic and Medicinal Chemistry, 2006, 14, 1462-1473.	1.4	41
85	Cocaine Esterase Prevents Cocaine-Induced Toxicity and the Ongoing Intravenous Self-Administration of Cocaine in Rats. Journal of Pharmacology and Experimental Therapeutics, 2009, 331, 445-455.	1.3	41
86	Molecular Mechanism of HIV-1 Tat Interacting with Human Dopamine Transporter. ACS Chemical Neuroscience, 2015, 6, 658-665.	1.7	41
87	Molecular Basis of the Selectivity of the Immunoproteasome Catalytic Subunit LMP2-Specific Inhibitor Revealed by Molecular Modeling and Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 12333-12339.	1.2	40
88	Kinetic characterization of high-activity mutants of human butyrylcholinesterase for the cocaine metabolite norcocaine. Biochemical Journal, 2014, 457, 197-206.	1.7	39
89	Theoretical Determination of Chromophores in the Chromogenic Effects of Aromatic Neurotoxicants. Journal of the American Chemical Society, 2002, 124, 2744-2752.	6.6	38
90	The gas and solution phase acidities of HNO, HOONO, HONO, and HONO2. International Journal of Mass Spectrometry, 2003, 227, 421-438.	0.7	38

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91	Theoretical Determination of Activation Free Energies for Alkaline Hydrolysis of Cyclic and Acyclic Phosphodiesters in Aqueous Solution. Journal of Physical Chemistry A, 2004, 108, 6407-6413.	1.1	38
92	Bioactive Permethrin/Î²-Cyclodextrin Inclusion Complex. Journal of Physical Chemistry B, 2006, 110, 7044-7048.	1.2	38
93	Rational Design, Preparation, and Characterization of a Therapeutic Enzyme Mutant with Improved Stability and Function for Cocaine Detoxification. ACS Chemical Biology, 2014, 9, 1764-1772.	1.6	37
94	Characterization of a Catalytic Ligand Bridging Metal Ions in Phosphodiesterases 4 and 5 by Molecular Dynamics Simulations and Hybrid Quantum Mechanical/Molecular Mechanical Calculations. Biophysical Journal, 2006, 91, 1858-1867.	0.2	36
95	Structural and functional characterization of human microsomal prostaglandin E synthase-1 by computational modeling and site-directed mutagenesis. Bioorganic and Medicinal Chemistry, 2006, 14, 3553-3562.	1.4	36
96	Formation and Stability of G-Quadruplexes Self-Assembled from Guanine-Rich Strands. Chemistry - A European Journal, 2007, 13, 945-949.	1.7	36
97	Fundamental Reaction Pathway for Peptide Metabolism by Proteasome: Insights from First-Principles Quantum Mechanical/Molecular Mechanical Free Energy Calculations. Journal of Physical Chemistry B, 2013, 117, 13418-13434.	1.2	36
98	Fundamental Reaction Pathway and Free Energy Profile for Butyrylcholinesterase-Catalyzed Hydrolysis of Heroin. Biochemistry, 2013, 52, 6467-6479.	1.2	35
99	Gene Transfer of Mutant Mouse Cholinesterase Provides High Lifetime Expression and Reduced Cocaine Responses with No Evident Toxicity. PLoS ONE, 2013, 8, e67446.	1.1	35
100	Fundamental Reaction Pathways and Free-Energy Barriers for Ester Hydrolysis of Intracellular Second-Messenger 3â€˜,5â€˜-Cyclic Nucleotide. Journal of Physical Chemistry A, 2004, 108, 3789-3797.	1.1	34
101	Reaction Pathway and Free Energy Profiles for Butyrylcholinesterase-Catalyzed Hydrolysis of Acetylthiocholine. Biochemistry, 2012, 51, 1297-1305.	1.2	34
102	Cyclic GMPâ€“mediated memory enhancement in the object recognition test by inhibitors of phosphodiesterase-2 in mice. Psychopharmacology, 2016, 233, 447-456.	1.5	34
103	Structure-based discovery of mPGES-1 inhibitors suitable for preclinical testing in wild-type mice as a new generation of anti-inflammatory drugs. Scientific Reports, 2018, 8, 5205.	1.6	34
104	Preparation and inÂvivo characterization of a cocaine hydrolase engineered from human butyrylcholinesterase for metabolizing cocaine. Biochemical Journal, 2013, 453, 447-454.	1.7	33
105	A quantitative LCâ€“MS/MS method for simultaneous determination of cocaine and its metabolites in whole blood. Journal of Pharmaceutical and Biomedical Analysis, 2017, 134, 243-251.	1.4	33
106	Talin2-mediated traction force drives matrix degradation and cell invasion. Journal of Cell Science, 2016, 129, 3661-3674.	1.2	32
107	Rational Redesign of Enzyme via the Combination of Quantum Mechanics/Molecular Mechanics, Molecular Dynamics, and Structural Biology Study. Journal of the American Chemical Society, 2021, 143, 15674-15687.	6.6	32
108	A Thermally Stable Form of Bacterial Cocaine Esterase: A Potential Therapeutic Agent for Treatment of Cocaine Abuse. Molecular Pharmacology, 2010, 77, 593-600.	1.0	31

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109	Substrate selectivity of high-activity mutants of human butyrylcholinesterase. Organic and Biomolecular Chemistry, 2013, 11, 7477.	1.5	31
110	Mccrearamycins Aâ€“D, Geldanamycinâ€Derived Cyclopentenone Macrolactams from an Eastern Kentucky Abandoned Coal Mine Microbe. Angewandte Chemie - International Edition, 2017, 56, 2994-2998.	7.2	31
111	Rational design of an enzyme mutant for anti-cocaine therapeutics. Journal of Computer-Aided Molecular Design, 2008, 22, 661-671.	1.3	30
112	Recent progress in protein drug design and discovery with a focus on novel approaches to the development of anticocaine medications. Future Medicinal Chemistry, 2009, 1, 515-528.	1.1	30
113	Why Does the G117H Mutation Considerably Improve the Activity of Human Butyrylcholinesterase against Sarin? Insights from Quantum Mechanical/Molecular Mechanical Free Energy Calculations. Biochemistry, 2012, 51, 8980-8992.	1.2	30
114	Fast Prediction of Binding Affinities of the SARS-CoV-2 Spike Protein Mutant N501Y (UK Variant) with ACE2 and Miniprotein Drug Candidates. Journal of Physical Chemistry B, 2021, 125, 4330-4336.	1.2	30
115	Microscopic Modes and Free Energies of 3-Phosphoinositide-Dependent Kinase-1 (PDK1) Binding with Celecoxib and Other Inhibitors. Journal of Physical Chemistry B, 2006, 110, 26365-26374.	1.2	29
116	Modeling Binding Modes of Î±7 Nicotinic Acetylcholine Receptor with Ligands: The Roles of Gln117 and Other Residues of the Receptor in Agonist Binding. Journal of Medicinal Chemistry, 2008, 51, 6293-6302.	2.9	29
117	Enzyme-therapy approaches for the treatment of drug overdose and addiction. Future Medicinal Chemistry, 2011, 3, 9-13.	1.1	29
118	Kinetic characterization of human butyrylcholinesterase mutants for the hydrolysis of cocaethylene. Biochemical Journal, 2014, 460, 447-457.	1.7	29
119	Mutations at Tyrosine 88, Lysine 92 and Tyrosine 470 of Human Dopamine Transporter Result in an Attenuation of HIV-1 Tat-Induced Inhibition of Dopamine Transport. Journal of NeuroImmune Pharmacology, 2015, 10, 122-135.	2.1	29
120	Plant-expressed cocaine hydrolase variants of butyrylcholinesterase exhibit altered allosteric effects of cholinesterase activity and increased inhibitor sensitivity. Scientific Reports, 2017, 7, 10419.	1.6	29
121	Bond strength and bond angles for hybrid orbitals composed of arbitrary sets of orbital angular momentum quantum number. International Journal of Quantum Chemistry, 1987, 32, 13-18.	1.0	28
122	First-principles studies of C-13 NMR chemical shift tensors of amino acids in crystal state. Computational and Theoretical Chemistry, 2004, 682, 73-82.	1.5	28
123	Human Microsomal Prostaglandin E Synthase-1 (mPGES-1) Binding with Inhibitors and the Quantitative Structureâ"Activity Correlation. Journal of Chemical Information and Modeling, 2008, 48, 179-185.	2.5	28
124	Reaction pathways and free energy profiles for cholinesterase-catalyzed hydrolysis of 6-monoacetylmorphine. Organic and Biomolecular Chemistry, 2014, 12, 2214-2227.	1.5	28
125	Fundamental reaction pathway and free energy profile of proteasome inhibition by syringolin A (SylA). Organic and Biomolecular Chemistry, 2015, 13, 6857-6865.	1.5	28
126	Computational neural network analysis of the affinity of lobeline and tetrabenazine analogs for the vesicular monoamine transporter-2. Bioorganic and Medicinal Chemistry, 2007, 15, 2975-2992.	1.4	27

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127	Modeling in vitro inhibition of butyrylcholinesterase using molecular docking, multi-linear regression and artificial neural network approaches. Bioorganic and Medicinal Chemistry, 2014, 22, 538-549.	1.4	27
128	Metabolic Enzymes of Cocaine Metabolite Benzoylecgonine. ACS Chemical Biology, 2016, 11, 2186-2194.	1.6	27
129	Role of glutamine 148 of human 15-hydroxyprostaglandin dehydrogenase in catalytic oxidation of prostaglandin E2. Bioorganic and Medicinal Chemistry, 2006, 14, 6486-6491.	1.4	26
130	Modeling Differential Binding of Î±4Î²2 Nicotinic Acetylcholine Receptor with Agonists and Antagonists. Journal of the American Chemical Society, 2008, 130, 16691-16696.	6.6	26
131	Reaction Pathway and Free Energy Profile for Cocaine Hydrolase-Catalyzed Hydrolysis of (â^')-Cocaine. Journal of Chemical Theory and Computation, 2012, 8, 1426-1435.	2.3	26
132	Crystal structure of Bacillus fastidious uricase reveals an unexpected folding of the C-terminus residues crucial for thermostability under physiological conditions. Applied Microbiology and Biotechnology, 2015, 99, 7973-7986.	1.7	26
133	Computational and Experimental Insights into the Mechanism of Substrate Recognition and Feedback Inhibition of Protoporphyrinogen Oxidase. PLoS ONE, 2013, 8, e69198.	1.1	26
134	Modeling and Re-Engineering of Azotobacter vinelandii Alginate Lyase to Enhance Its Catalytic Efficiency for Accelerating Biofilm Degradation. PLoS ONE, 2016, 11, e0156197.	1.1	26
135	Computational characterization of how the VX nerve agent binds human serum paraoxonase 1. Journal of Molecular Modeling, 2011, 17, 97-109.	0.8	25
136	Reaction Pathways and Free Energy Barriers for Alkaline Hydrolysis of Insecticide 2-Trimethylammonioethyl Methylphosphonofluoridate and Related Organophosphorus Compounds:Â Electrostatic and Steric Effects. Journal of Organic Chemistry, 2004, 69, 8451-8458.	1.7	24
137	Clinical Potential of an Enzyme-based Novel Therapy for Cocaine Overdose. Scientific Reports, 2017, 7, 15303.	1.6	24
138	Computational Determination of Binding Structures and Free Energies of Phosphodiesterase-2 with Benzo[1,4]diazepin-2-one Derivatives. Journal of Physical Chemistry B, 2010, 114, 16020-16028.	1.2	23
139	Free Energy Perturbation Simulation on Transition States and High-Activity Mutants of Human Butyrylcholinesterase for (â^')-Cocaine Hydrolysis. Journal of Physical Chemistry B, 2010, 114, 10889-10896.	1.2	23
140	Understanding Microscopic Binding of Human Microsomal Prostaglandin E Synthase-1 with Substrates and Inhibitors by Molecular Modeling and Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 7320-7329.	1.2	22
141	Theoretical studies of nonenzymatic reaction pathways for the three reaction stages of the carboxylation of ribulose-1,5-bisphosphate. Perkin Transactions II RSC, 2001, , 23-29.	1.1	21
142	Computational Insights into the Chemical Structures and Mechanisms of the Chromogenic and Neurotoxic Effects of Aromatic Î³-diketones. Journal of Physical Chemistry B, 2003, 107, 2853-2861.	1.2	21
143	Fundamental Reaction Pathway and Free Energy Profile for Hydrolysis of Intracellular Second Messenger Adenosine 3â€²,5â€²-Cyclic Monophosphate (cAMP) Catalyzed by Phosphodiesterase-4. Journal of Physical Chemistry B, 2011, 115, 12208-12219.	1.2	21
144	Reaction pathways and free energy profiles for spontaneous hydrolysis of urea and tetramethylurea: unexpected substituent effects. Organic and Biomolecular Chemistry, 2013, 11, 7595.	1.5	21

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145	Influence of Sugar Amine Regiochemistry on Digitoxigenin Neoglycoside Anticancer Activity. ACS Medicinal Chemistry Letters, 2015, 6, 1053-1058.	1.3	21
146	Catalytic Reaction Mechanism for Drug Metabolism in Human Carboxylesterase-1: Cocaine Hydrolysis Pathway. Molecular Pharmaceutics, 2018, 15, 3871-3880.	2.3	21
147	Maximum overlap symmetry orbitals. International Journal of Quantum Chemistry, 1991, 39, 729-746.	1.0	20
148	Maximum bond order hybrid orbitals. Theoretica Chimica Acta, 1993, 84, 511-520.	0.9	20
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