Fang Zheng

List of Publications by Year
in descending order

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97 papers	2,327 citations	186265 28 h-index	243625 44 g-index
100 all docs	100 docs citations	100 times ranked	1780 citing authors

#	Article	IF	Citations
1	Cocaine hydrolase blocks cocaineâ€induced dopamine transporter trafficking to the plasma membrane. Addiction Biology, 2022, 27, e13089.	2.6	8
2	Recovery of dopaminergic system after cocaine exposure and impact of a longâ€acting cocaine hydrolase. Addiction Biology, 2022, 27, .	2.6	6
3	Development of a Highly Efficient Long-Acting Cocaine Hydrolase Entity to Accelerate Cocaine Metabolism. Bioconjugate Chemistry, 2022, 33, 1340-1349.	3.6	9
4	Systematic Structure-Based Virtual Screening Approach to Antibody Selection and Design of a Humanized Antibody against Multiple Addictive Opioids without Affecting Treatment Agents Naloxone and Naltrexone. ACS Chemical Neuroscience, 2021, 12, 184-194.	3.5	2
5	Clinical data mining reveals analgesic effects of lapatinib in cancer patients. Scientific Reports, 2021, 11, 3528.	3.3	1
6	Reengineering of Albumin-Fused Cocaine Hydrolase CocH1 (TV-1380) to Prolong Its Biological Half-Life. AAPS Journal, 2020, 22, 5.	4.4	9
7	Effects of Cebranopadol on Cocaine-induced Hyperactivity and Cocaine Pharmacokinetics in Rats. Scientific Reports, 2020, 10, 9254.	3.3	10
8	Clinical potential of a rationally engineered enzyme for treatment of cocaine dependence: Long-lasting blocking of the psychostimulant, discriminative stimulus, and reinforcing effects of cocaine. Neuropharmacology, 2020, 176, 108251.	4.1	12
9	Efficient Cocaine Degradation by Cocaine Esterase-Loaded Red Blood Cells. Frontiers in Physiology, 2020, 11, 573492.	2.8	1
10	Structure-Based Design and Discovery of a Long-Acting Cocaine Hydrolase Mutant with Improved Binding Affinity to Neonatal Fc Receptor for Treatment of Cocaine Abuse. AAPS Journal, 2020, 22, 62.	4.4	12
11	DREAM-in-CDM Approach and Identification of a New Generation of Anti-inflammatory Drugs Targeting mPGES-1. Scientific Reports, 2020, 10, 10187.	3.3	13
12	Catalytic activities of cocaine hydrolases against the most toxic cocaine metabolite norcocaethylene. Organic and Biomolecular Chemistry, 2020, 18, 1968-1977.	2.8	12
13	Cebranopadol reduces cocaine self-administration in male rats: Dose, treatment and safety consideration. Neuropharmacology, 2020, 172, 108128.	4.1	6
14	In Silico Observation of the Conformational Opening of the Glutathione-Binding Site of Microsomal Prostaglandin E2 Synthase-1. Journal of Chemical Information and Modeling, 2019, 59, 3839-3845.	5.4	6
15	Dimerization of human butyrylcholinesterase expressed in bacterium for development of a thermally stable bioscavenger of organophosphorus compounds. Chemico-Biological Interactions, 2019, 310, 108756.	4.0	4
16	PEGylation but Not Fc-Fusion Improves in Vivo Residence Time of a Thermostable Mutant of Bacterial Cocaine Esterase. Bioconjugate Chemistry, 2019, 30, 3021-3027.	3.6	2
17	Development of a novel prostate apoptosis response-4 (Par-4) protein entity with an extended duration of action for therapeutic treatment of cancer. Protein Engineering, Design and Selection, 2019, 32, 159-166.	2.1	6
18	In vivo characterization of toxicity of norcocaethylene and norcocaine identified as the most toxic cocaine metabolites in male mice. Drug and Alcohol Dependence, 2019, 204, 107462.	3.2	14

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19	Structure-based virtual screening leading to discovery of highly selective butyrylcholinesterase inhibitors with solanaceous alkaloid scaffolds. Chemico-Biological Interactions, 2019, 308, 372-376.	4.0	12
20	Development of a long-acting Fc-fused cocaine hydrolase with improved yield of protein expression. Chemico-Biological Interactions, 2019, 306, 89-95.	4.0	17
21	Development of Fc-Fused Cocaine Hydrolase for Cocaine Addiction Treatment: Catalytic and Pharmacokinetic Properties. AAPS Journal, 2018, 20, 53.	4.4	13
22	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.	3.3	34
23	Design, synthesis, and discovery of 5-((1,3-diphenyl-1 H -pyrazol-4-yl)methylene)pyrimidine-2,4,6(1 H ,3 H ,5) Tj ETQq1 1 0.784314 rgBT Letters, 2018, 28, 858-862.	2.2	11
24	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.	4.4	50
25	Effectiveness of a Cocaine Hydrolase for Cocaine Toxicity Treatment in Male and Female Rats. AAPS Journal, 2018, 20, 3.	4.4	15
26	Blocking drug activation as a therapeutic strategy to attenuate acute toxicity and physiological effects of heroin. Scientific Reports, 2018, 8, 16762.	3.3	8
27	Oligomerization and Catalytic Parameters of Human UDP-Glucuronosyltransferase 1A10: Expression and Characterization of the Recombinant Protein. Drug Metabolism and Disposition, 2018, 46, 1446-1452.	3.3	2
28	Kinetic characterization of cholinesterases and a therapeutically valuable cocaine hydrolase for their catalytic activities against heroin and its metabolite 6-monoacetylmorphine. Chemico-Biological Interactions, 2018, 293, 107-114.	4.0	10
29	Catalytic Reaction Mechanism for Drug Metabolism in Human Carboxylesterase-1: Cocaine Hydrolysis Pathway. Molecular Pharmaceutics, 2018, 15, 3871-3880.	4.6	21
30	Clinical Potential of an Enzyme-based Novel Therapy for Cocaine Overdose. Scientific Reports, 2017, 7, 15303.	3.3	24
31	Selective inhibitors of human mPGES-1 from structure-based computational screening. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 3739-3743.	2.2	13
32	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.	2.8	33
33	Feature Guided In-Situ Indices Generation and Data Placement on Distributed Deep Memory Hierarchies. , 2017, , .		0
34	Actions of Butyrylcholinesterase Against Cocaine. , 2017, , 663-672.		3
35	Reply to Curry and Coombs: Benzoic acid is formed predominantly from the benzoyl ester hydrolysis in the presence of cocaine hydrolase. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E2102-E2103.	7.1	0
36	Unexpected Reaction Pathway for butyrylcholinesterase-catalyzed inactivation of â€œhunger hormoneâ€• ghrelin. Scientific Reports, 2016, 6, 22322.	3.3	13

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37	Effects of a cocaine hydrolase engineered from human butyrylcholinesterase on metabolic profile of cocaine in rats. Chemico-Biological Interactions, 2016, 259, 104-109.	4.0	7
38	Free energy profiles of cocaine esterase-cocaine binding process by molecular dynamics and potential of mean force simulations. Chemico-Biological Interactions, 2016, 259, 142-147.	4.0	1
39	Potential anti-obesity effects of a long-acting cocaine hydrolase. Chemico-Biological Interactions, 2016, 259, 99-103.	4.0	5
40	Plant expression of cocaine hydrolase-Fc fusion protein for treatment of cocaine abuse. BMC Biotechnology, 2016, 16, 72.	3.3	5
41	Reaction pathway for cocaine hydrolase-catalyzed hydrolysis of (+)-cocaine. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	2
42	Metabolic Enzymes of Cocaine Metabolite Benzoylecgonine. ACS Chemical Biology, 2016, 11, 2186-2194.	3.4	27
43	Long-acting cocaine hydrolase for addiction therapy. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 422-427.	7.1	56
44	Cocaine Hydrolases Designed from Butyrylcholinesterase. , 2016, , 187-225.		5
45	Kinetic characterization of a cocaine hydrolase engineered from mouse butyrylcholinesterase. Biochemical Journal, 2015, 466, 243-251.	3.7	16
46	Nanostructured lipid carriers for oral delivery of baicalin: In vitro and in vivo evaluation. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2015, 466, 154-159.	4.7	59
47	Kinetic characterization of high-activity mutants of human butyrylcholinesterase for the cocaine metabolite norcocaine. Biochemical Journal, 2014, 457, 197-206.	3.7	39
48	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.	3.0	27
49	Kinetic characterization of human butyrylcholinesterase mutants for the hydrolysis of cocaethylene. Biochemical Journal, 2014, 460, 447-457.	3.7	29
50	A model of glycosylated human butyrylcholinesterase. Molecular BioSystems, 2014, 10, 348-354.	2.9	7
51	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.	3.4	37
52	A highly efficient cocaine-detoxifying enzyme obtained by computational design. Nature Communications, 2014, 5, 3457.	12.8	67
53	Amino-acid mutations to extend the biological half-life of a therapeutically valuable mutant of human butyrylcholinesterase. Chemico-Biological Interactions, 2014, 214, 18-25.	4.0	14
54	Catalytic activities of a cocaine hydrolase engineered from human butyrylcholinesterase against (+)- and (â^')-cocaine. Chemico-Biological Interactions, 2013, 203, 57-62.	4.0	16

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55	Substrate selectivity of high-activity mutants of human butyrylcholinesterase. Organic and Biomolecular Chemistry, 2013, 11, 7477.	2.8	31
56	Binding structures and energies of the human neonatal Fc receptor with human Fc and its mutants by molecular modeling and dynamics simulations. Molecular BioSystems, 2013, 9, 3047.	2.9	14
57	Computational Modeling of Solvent Effects on Protein-Ligand Interactions Using Fully Polarizable Continuum Model and Rational Drug Design. Communications in Computational Physics, 2013, 13, 31-60.	1.7	8
58	Improving the inhibitory activity of arylidenaminoguanidine compounds at the N-methyl-d-aspartate receptor complex from a recursive computational-experimental structureâ€“activity relationship study. Bioorganic and Medicinal Chemistry, 2013, 21, 1764-1774.	3.0	11
59	Preparation and inÂvivo characterization of a cocaine hydrolase engineered from human butyrylcholinesterase for metabolizing cocaine. Biochemical Journal, 2013, 453, 447-454.	3.7	33
60	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.	3.2	43
61	Are pharmacokinetic approaches feasible for treatment of cocaine addiction and overdose?. Future Medicinal Chemistry, 2012, 4, 125-128.	2.3	52
62	Cocaine Esteraseâ€“Cocaine Binding Process and the Free Energy Profiles by Molecular Dynamics and Potential of Mean Force Simulations. Journal of Physical Chemistry B, 2012, 116, 3361-3368.	2.6	13
63	Enzyme-therapy approaches for the treatment of drug overdose and addiction. Future Medicinal Chemistry, 2011, 3, 9-13.	2.3	29
64	Human Butyrylcholinesteraseâ€“Cocaine Binding Pathway and Free Energy Profiles by Molecular Dynamics and Potential of Mean Force Simulations. Journal of Physical Chemistry B, 2011, 115, 11254-11260.	2.6	12
65	Design, Synthesis and Interaction at the Vesicular Monoamine Transporter-2 of Lobeline Analogs: Potential Pharmacotherapies for the Treatment of Psychostimulant Abuse. Current Topics in Medicinal Chemistry, 2011, 11, 1103-1127.	2.1	17
66	Design, Preparation, and Characterization of High-Activity Mutants of Human Butyrylcholinesterase Specific for Detoxification of Cocaine. Molecular Pharmacology, 2011, 79, 290-297.	2.3	81
67	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.	2.6	23
68	Design of High-Activity Mutants of Human Butyrylcholinesterase against (â^')-Cocaine: Structural and Energetic Factors Affecting the Catalytic Efficiency. Biochemistry, 2010, 49, 9113-9119.	2.5	44
69	Reaction Pathway and Free Energy Profile for Prechemical Reaction Step of Human Butyrylcholinesterase-Catalyzed Hydrolysis of (â^')-Cocaine by Combined Targeted Molecular Dynamics and Potential of Mean Force Simulations. Journal of Physical Chemistry B, 2010, 114, 13545-13554.	2.6	13
70	Computational neural network analysis of the affinity of N-n-alkylnicotinium salts for the Î±4Î²2* nicotinic acetylcholine receptor. Journal of Enzyme Inhibition and Medicinal Chemistry, 2009, 24, 157-168.	5.2	7
71	First-principles determination of molecular conformations of indolizidine (â^')-235Bâ€² in solution. Theoretical Chemistry Accounts, 2009, 124, 269-278.	1.4	3
72	QSAR study on maximal inhibition (Imax) of quaternary ammonium antagonists for S-(â^')-nicotine-evoked dopamine release from dopaminergic nerve terminals in rat striatum. Bioorganic and Medicinal Chemistry, 2009, 17, 4477-4485.	3.0	8

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73	Free-Energy Perturbation Simulation on Transition States and Redesign of Butyrylcholinesterase. Biophysical Journal, 2009, 96, 1931-1938.	0.5	58
74	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.	2.3	30
75	Rational design of an enzyme mutant for anti-cocaine therapeutics. Journal of Computer-Aided Molecular Design, 2008, 22, 661-671.	2.9	30
76	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.	6.4	29
77	Structure-and-mechanism-based design and discovery of therapeutics for cocaine overdose and addiction. Organic and Biomolecular Chemistry, 2008, 6, 836-843.	2.8	46
78	Most Efficient Cocaine Hydrolase Designed by Virtual Screening of Transition States. Journal of the American Chemical Society, 2008, 130, 12148-12155.	13.7	164
79	Modeling Differential Binding of Î±4Î²2 Nicotinic Acetylcholine Receptor with Agonists and Antagonists. Journal of the American Chemical Society, 2008, 130, 16691-16696.	13.7	26
80	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.	3.0	27
81	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.	6.4	46
82	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.	3.0	53
83	Electrical Properties of Laser-Synthesized Aluminum Oxide-Tungsten Oxide Ceramics. Journal of the American Ceramic Society, 2005, 81, 2443-2448.	3.8	1
84	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.	13.7	46
85	Large-scale simulations of cellular signaling processes. Parallel Computing, 2004, 30, 1137-1149.	2.1	10
86	Electron Affinities of Aln Clusters and Multiple-Fold Aromaticity of the Square Al42- Structure. ChemInform, 2003, 34, no.	0.0	0
87	Fundamental Reaction Mechanism for Cocaine Hydrolysis in Human Butyrylcholinesterase. Journal of the American Chemical Society, 2003, 125, 2462-2474.	13.7	131
88	Theoretical Determination of Two Structural Forms of the Active Site in Cadmium-Containing Phosphotriesterases. Journal of Physical Chemistry B, 2002, 106, 717-722.	2.6	45
89	Electron Affinities of AlnClusters and Multiple-Fold Aromaticity of the Square Al42-Structure. Journal of the American Chemical Society, 2002, 124, 14795-14803.	13.7	162
90	First Computational Evidence for a Catalytic Bridging Hydroxide Ion in a Phosphodiesterase Active Site. Journal of the American Chemical Society, 2001, 123, 2835-2838.	13.7	69

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91	Quantum chemical definition and calculation of oxidation number. Computational and Theoretical Chemistry, 1994, 309, 309-314.	1.5	3
92	Band structure and density of states of NaxWO3. Computational and Theoretical Chemistry, 1993, 285, 89-98.	1.5	11
93	Analysis of aluminum tungsten oxide ceramics synthesized by a highâ€power cw CO2laser. Journal of Applied Physics, 1993, 74, 1616-1624.	2.5	4
94	The canonical orthogonalization of AO basis set and block diagonalization of the hamiltonian matrix. Computational and Theoretical Chemistry, 1991, 226, 339-349.	1.5	9
95	Maximum overlap symmetry orbitals. International Journal of Quantum Chemistry, 1991, 39, 729-746.	2.0	20
96	An improved iterative maximum overlap approximation method. Computational and Theoretical Chemistry, 1990, 205, 267-277.	1.5	14
97	Calculation of the maximum bond order. Theoretica Chimica Acta, 1990, 78, 129-131.	0.8	20