Xiaoqin Huang

List of Publications by Year
in descending order

23 papers	649 citations	567281 15 h-index	642732 23 g-index
23 all docs	23 docs citations	23 times ranked	767 citing authors

#	Article	IF	Citations
1	How Dopamine Transporter Interacts with Dopamine: Insights from Molecular Modeling and Simulation. Biophysical Journal, 2007, 93, 3627-3639.	0.5	79
2	Mechanism for Cocaine Blocking the Transport of Dopamine: Insights from Molecular Modeling and Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 15057-15066.	2.6	72
3	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.	11.2	71
4	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
5	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
6	Molecular Mechanism of HIV-1 Tat Interacting with Human Dopamine Transporter. ACS Chemical Neuroscience, 2015, 6, 658-665.	3.5	41
7	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.	3.0	36
8	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
9	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
10	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
11	Modeling and Re-Engineering of Azotobacter vinelandii Alginate Lyase to Enhance Its Catalytic Efficiency for Accelerating Biofilm Degradation. PLoS ONE, 2016, 11, e0156197.	2.5	26
12	Computational design of a thermostable mutant of cocaine esterase via molecular dynamics simulations. Organic and Biomolecular Chemistry, 2011, 9, 4138.	2.8	20
13	Binding free energies for nicotine analogs inhibiting cytochrome P450 2A6 by a combined use of molecular dynamics simulations and QM/MM-PBSA calculations. Bioorganic and Medicinal Chemistry, 2014, 22, 2149-2156.	3.0	17
14	Computational modeling of human dopamine transporter structures, mechanism and its interaction with HIV-1 transactivator of transcription. Future Medicinal Chemistry, 2016, 8, 2077-2089.	2.3	17
15	Kinetic characterization of a cocaine hydrolase engineered from mouse butyrylcholinesterase. Biochemical Journal, 2015, 466, 243-251.	3.7	16
16	Microscopic Binding of M5 Muscarinic Acetylcholine Receptor with Antagonists by Homology Modeling, Molecular Docking, and Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2012, 116, 532-541.	2.6	14
17	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
18	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

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19	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
20	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
21	Molecular modeling and redesign of alginate lyase from Pseudomonas aeruginosa for accelerating CRPA biofilm degradation. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1875-1887.	2.6	11
22	Design, synthesis, and biological activity of 5â€²-phenyl-1,2,5,6-tetrahydro-3,3â€²-bipyridine analogues as potential antagonists of nicotinic acetylcholine receptors. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 4350-4353.	2.2	2
23	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