Xianqiang Sun

List of Publications by Year in descending order

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Version: 2024-02-01

21	504	623734	713466
papers	citations	14 h-index	21 g-index

24	24	24	929
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Atomistic and Thermodynamic Analysis of N6-Methyladenosine (m⁶A) Recognition by the Reader Domain of YTHDC1. Journal of Chemical Theory and Computation, 2021, 17, 1240-1249.	5.3	18
2	Molecular insights into ago-allosteric modulation of the human glucagon-like peptide-1 receptor. Nature Communications, 2021, 12, 3763.	12.8	41
3	Structural insights into the activation of GLP-1R by a small molecule agonist. Cell Research, 2020, 30, 1140-1142.	12.0	29
4	Choice of Adaptive Sampling Strategy Impacts State Discovery, Transition Probabilities, and the Apparent Mechanism of Conformational Changes. Journal of Chemical Theory and Computation, 2018, 14, 5459-5475.	5.3	55
5	Simulation of spontaneous G protein activation reveals a new intermediate driving GDP unbinding. ELife, 2018, 7, .	6.0	39
6	Propagation of the Allosteric Modulation Induced by Sodium in the Î´â€Opioid Receptor. Chemistry - A European Journal, 2017, 23, 4615-4624.	3.3	20
7	Allosteric inhibitor remotely modulates the conformation of the orthestric pockets in mutant IDH2/R140Q. Scientific Reports, 2017, 7, 16458.	3.3	18
8	Structure and Dynamics of PD-L1 and an Ultra-High-Affinity PD-1 Receptor Mutant. Structure, 2016, 24, 1719-1728.	3.3	86
9	Computational investigation of the interaction mechanism between the estrogen related receptor Î± and its agonists. RSC Advances, 2016, 6, 94119-94127.	3.6	6
10	Molecular switches of the Î¼ opioid receptor triggered by 6â€²-GNTI and 5â€²-GNTI. Scientific Reports, 2016, 6, 18913.	3.3	19
11	Computational insight into conformational states of glucagon-like peptide-1 receptor (GLP-1R) and its binding mode with GLP-1. RSC Advances, 2016, 6, 13490-13497.	3.6	6
12	Residues remote from the binding pocket control the antagonist selectivity towards the corticotropin-releasing factor receptor-1. Scientific Reports, 2015, 5, 8066.	3.3	17
13	Synthesis, structureâ€“activity relationship and biological evaluation of novel arylpiperzines as Î±1A/1D-AR subselective antagonists for BPH. Bioorganic and Medicinal Chemistry, 2015, 23, 7735-7742.	3.0	15
14	Microsecond Molecular Dynamics Simulations Provide Insight into the Allosteric Mechanism of the Gs Protein Uncoupling from the Î²2Adrenergic Receptor. Journal of Physical Chemistry B, 2014, 118, 141212122505008.	2.6	10
15	Functional Water Molecules in Rhodopsin Activation. Journal of Physical Chemistry B, 2014, 118, 10863-10873.	2.6	34
16	Non-antibiotic agent ginsenoside 20(S)-Rh2 enhanced the antibacterial effects of ciprofloxacin in vitro and in vivo as a potential NorA inhibitor. European Journal of Pharmacology, 2014, 740, 277-284.	3.5	32
17	Inhibitors of HIVâ€1 Integraseâ€Human LEDGF/p75 Interaction Identified from Natural Products via Virtual Screening. Chinese Journal of Chemistry, 2012, 30, 2752-2758.	4.9	2
18	In silico investigation of interactions between human cannabinoid receptor-1 and its antagonists. Journal of Molecular Modeling, 2012, 18, 3831-3845.	1.8	6

#	Article	IF	Citations
19	Identification of old drugs as potential inhibitors of HIV-1 integrase â€“ human LEDGF/p75 interaction via molecular docking. Journal of Molecular Modeling, 2012, 18, 4995-5003.	1.8	21
20	Insights into the binding modes of human Î²3-adrenergic receptor agonists with ligand-based and receptor-based methods. Molecular Diversity, 2011, 15, 817-831.	3.9	10
21	Computational investigation of interactions between human H2 receptor and its agonists. Journal of Molecular Graphics and Modelling, 2011, 29, 693-701.	2.4	17