

Hanxun Wang

List of Publications by Year in descending order

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Version: 2024-02-01

20
papers

213
citations

1307594

7
h-index

1058476

14
g-index

20
all docs

20
docs citations

20
times ranked

268
citing authors

#	ARTICLE	IF	CITATIONS
1	Identification of the active compounds and their mechanisms of medicinal and edible Shanzha based on network pharmacology and molecular docking. <i>Journal of Food Biochemistry</i> , 2022, 46, e14020.	2.9	7
2	Role of polymers in the physical and chemical stability of amorphous solid dispersion: A case study of carbamazepine. <i>European Journal of Pharmaceutical Sciences</i> , 2022, 169, 106086.	4.0	18
3	Discovery of benzo[d]isothiazole derivatives as novel scaffold inhibitors targeting the programmed cell death-1/programmed cell death-ligand 1 (PD-1/PD-L1) interaction through "ring fusion" strategy. <i>Bioorganic Chemistry</i> , 2022, 123, 105769.	4.1	6
4	Discovery of small molecule inhibitors through pharmacophore modeling, molecular docking, molecular dynamics simulation and experimental validation against myeloid cell leukemia-1 (Mcl-1). <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 2512-2525.	3.5	7
5	Molecular docking, 3D-QSAR, and molecular dynamics simulations of thieno[3,2-b]pyrrole derivatives against anticancer targets of KDM1A/LSD1. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 1189-1202.	3.5	21
6	Structural basis for tailor-made selective PI3K $\hat{\gamma}$ inhibitors: a computational perspective. <i>New Journal of Chemistry</i> , 2021, 45, 373-382.	2.8	4
7	Sacubitril-valsartan cocrystal revisited: role of polymer excipients in the formulation. <i>Expert Opinion on Drug Delivery</i> , 2021, 18, 515-526.	5.0	11
8	Drug discovery targeting p21-activated kinase 4 (PAK4): a patent review. <i>Expert Opinion on Therapeutic Patents</i> , 2021, 31, 977-987.	5.0	8
9	Intermolecular insights into allosteric inhibition of histone lysine-specific demethylase 1. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2021, 1865, 129990.	2.4	6
10	Development, Physical-Chemical Characterization, and Molecular Docking Simulations of Ursolic Acid-Sodium Alginate Complexes. <i>Journal of Agricultural and Food Chemistry</i> , 2021, 69, 14311-14319.	5.2	3
11	In silico studies on p21-activated kinase 4 inhibitors: comprehensive application of 3D-QSAR analysis, molecular docking, molecular dynamics simulations, and MM-GBSA calculation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 4119-4133.	3.5	13
12	Precise design of highly isoform-selective p21-activated kinase 4 inhibitors: computational insights into the selectivity mechanism through molecular dynamics simulation and binding free energy calculation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 3825-3837.	3.5	8
13	PB-10, a thiazolo[4,5-d] pyrimidine derivative, targets p21-activated kinase 4 in human colorectal cancer cells. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2020, 30, 126807.	2.2	9
14	Computational investigation reveals Picrasidine C as selective PPAR γ lead: binding pattern, selectivity mechanism and ADME/tox profile. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 5401-5418.	3.5	8
15	Homology modeling, molecular dynamics and virtual screening of endothelin-A receptor for the treatment of pulmonary arterial hypertension. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 39, 1-12.	3.5	6
16	Structure-based virtual screening of natural products as potential stearyl-coenzyme a desaturase 1 (SCD1) inhibitors. <i>Computational Biology and Chemistry</i> , 2020, 86, 107263.	2.3	5
17	In vivo irreversible albumin-binding near-infrared dye conjugate as a naked-eye and fluorescence dual-mode imaging agent for lymph node tumor metastasis diagnosis. <i>Biomaterials</i> , 2019, 217, 119279.	11.4	39
18	Quinone-thioether metabolites of hydroquinone play a dual role in promoting a vicious cycle of ROS generation: in vitro and in silico insights. <i>Archives of Toxicology</i> , 2019, 93, 1297-1309.	4.2	12

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19	Molecular dynamics simulation and QM/MM calculation reveal the selectivity mechanism of type I 1/2 kinase inhibitors: the effect of intramolecular H-bonds and conformational restriction for improved selectivity. Physical Chemistry Chemical Physics, 2019, 21, 24147-24164.	2.8	21
20	Computational Strategy Revealing the Structural Determinant of Ligand Selectivity towards Highly Similar Protein Targets. Current Drug Targets, 2019, 21, 76-88.	2.1	1