Hanxun Wang

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2940624/publications.pdf

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20	213	1307594	1058476
papers	citations	7	14
		h-index	g-index

20	20	20	268
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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. Biomaterials, 2019, 217, 119279.	11.4	39
2	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
3	Molecular docking, 3D-QSAR, and molecular dynamics simulations of thieno[3,2-b]pyrrole derivatives against anticancer targets of KDM1A/LSD1. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1189-1202.	3.5	21
4	Role of polymers in the physical and chemical stability of amorphous solid dispersion: A case study of carbamazepine. European Journal of Pharmaceutical Sciences, 2022, 169, 106086.	4.0	18
5	In silico studies on p21-activated kinase 4 inhibitors: comprehensive application of 3D-QSAR analysis, molecular docking, molecular dynamics simulations, and MM-GBSA calculation. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4119-4133.	3.5	13
6	Quinoneâ€“thioether metabolites of hydroquinone play a dual role in promoting a vicious cycle of ROS generation: in vitro and in silico insights. Archives of Toxicology, 2019, 93, 1297-1309.	4.2	12
7	Sacubitril-valsartan cocrystal revisited: role of polymer excipients in the formulation. Expert Opinion on Drug Delivery, 2021, 18, 515-526.	5.0	11
8	PB-10, a thiazolo[4,5-d] pyrimidine derivative, targets p21-activated kinase 4 in human colorectal cancer cells. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 126807.	2.2	9
9	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. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3825-3837.	3.5	8
10	Computational investigation reveals Picrasidine C as selective PPARÎ± lead: binding pattern, selectivity mechanism and ADME/tox profile. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5401-5418.	3.5	8
11	Drug discovery targeting p21-activated kinase 4 (PAK4): a patent review. Expert Opinion on Therapeutic Patents, 2021, 31, 977-987.	5.0	8
12	Discovery of small molecule inhibitors through pharmacophore modeling, molecular docking, molecular dynamics simulation and experimental validation against myeloid cell leukemia-1 (Mcl-1). Journal of Biomolecular Structure and Dynamics, 2021, 39, 2512-2525.	3.5	7
13	Identification of the active compounds and their mechanisms of medicinal and edible Shanzha based on network pharmacology and molecular docking. Journal of Food Biochemistry, 2022, 46, e14020.	2.9	7
14	Homology modeling, molecular dynamics and virtual screening of endothelin-A receptor for the treatment of pulmonary arterial hypertension. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-12.	3.5	6
15	Intermolecular insights into allosteric inhibition of histone lysine-specific demethylase 1. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129990.	2.4	6
16	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 â€œring fusionâ€•strategy. Bioorganic Chemistry, 2022, 123, 105769.	4.1	6
17	Structure-based virtual screening of natural products as potential stearoyl-coenzyme a desaturase 1 (SCD1) inhibitors. Computational Biology and Chemistry, 2020, 86, 107263.	2.3	5
18	Structural basis for tailor-made selective PI3K Î±/Î² inhibitors: a computational perspective. New Journal of Chemistry, 2021, 45, 373-382.	2.8	4

#	Article	IF	Citations
19	Development, Physicalâ€“Chemical Characterization, and Molecular Docking Simulations of Ursolic Acidâ€“Sodium Alginate Complexes. Journal of Agricultural and Food Chemistry, 2021, 69, 14311-14319.	5.2	3
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