Shiliang Wu

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9520500/publications.pdf

Version: 2024-02-01

8 papers	62 citations	1684188 5 h-index	1588992 8 g-index
8 all docs	8 docs citations	8 times ranked	42 citing authors

#	Article	IF	Citations
1	Revealing binding selectivity of inhibitors toward bromodomain-containing proteins 2 and 4 using multiple short molecular dynamics simulations and free energy analyses. SAR and QSAR in Environmental Research, 2020, 31, 373-398.	2.2	16
2	Probing molecular mechanism of inhibitor bindings to bromodomain-containing protein 4 based on molecular dynamics simulations and principal component analysis. SAR and QSAR in Environmental Research, 2020, 31, 547-570.	2.2	14
3	Binding selectivity of inhibitors toward the first over the second bromodomain of BRD4: theoretical insights from free energy calculations and multiple short molecular dynamics simulations. RSC Advances, 2021, 11, 745-759.	3.6	11
4	Insights into interaction mechanism of inhibitors E3T, E3H and E3B with CREB binding protein by using molecular dynamics simulations and MM-GBSA calculations. SAR and QSAR in Environmental Research, 2021, 32, 221-246.	2.2	9
5	Decoding molecular mechanism underlying binding of drugs to HIV-1 protease with molecular dynamics simulations and MM-GBSA calculations. SAR and QSAR in Environmental Research, 2021, 32, 889-915.	2.2	6
6	Insights into effect of the Asp25/Asp25Ê¹ protonation states on binding of inhibitors Amprenavir and MKP97 to HIV-1 protease using molecular dynamics simulations and MM-GBSA calculations. SAR and QSAR in Environmental Research, 2021, 32, 615-641.	2.2	3
7	Molecular dynamics insights into binding selectivity of inhibitors toward BRD4 and CBP. Chemical Physics Letters, 2021, 769, 138435.	2.6	2
8	Molecular dynamics simulations data of six compounds F3J-BRD4/CBP, EX1-BRD4/CBP, and E2T-BRD4/CBP. Data in Brief, 2021, 36, 107009.	1.0	1