Tailong Lei

List of Publications by Year in descending order

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840776 1199594 12 635 11 12 citations h-index g-index papers 12 12 12 744 citing authors docs citations times ranked all docs

#	Article	IF	CITATIONS
1	Do we need different machine learning algorithms for QSAR modeling? A comprehensive assessment of 16 machine learning algorithms on 14 QSAR data sets. Briefings in Bioinformatics, 2021, 22, .	6.5	70
2	ADMET evaluation in drug discovery. 20. Prediction of breast cancer resistance protein inhibition through machine learning. Journal of Cheminformatics, 2020, 12, 16.	6.1	45
3	ADMET Evaluation in Drug Discovery. 19. Reliable Prediction of Human Cytochrome P450 Inhibition Using Artificial Intelligence Approaches. Journal of Chemical Information and Modeling, 2019, 59, 4587-4601.	5.4	85
4	Importance of Incorporating Protein Flexibility in Molecule Modeling: A Theoretical Study on Type $11/2$ NIK Inhibitors. Frontiers in Pharmacology, 2019, 10, 345.	3.5	11
5	farPPI: a webserver for accurate prediction of protein-ligand binding structures for small-molecule PPI inhibitors by MM/PB(GB)SA methods. Bioinformatics, 2019, 35, 1777-1779.	4.1	59
6	Reliability of Docking-Based Virtual Screening for GPCR Ligands with Homology Modeled Structures: A Case Study of the Angiotensin II Type I Receptor. ACS Chemical Neuroscience, 2019, 10, 677-689.	3.5	23
7	Importance of protein flexibility on molecular recognition: modeling binding mechanisms of aminopyrazine inhibitors to Nek2. Physical Chemistry Chemical Physics, 2018, 20, 5591-5605.	2.8	15
8	Comprehensive assessment of nine docking programs on type II kinase inhibitors: prediction accuracy of sampling power, scoring power and screening power. Briefings in Bioinformatics, 2018, , .	6.5	16
9	Assessing the performance of MM/PBSA and MM/GBSA methods. 8. Predicting binding free energies and poses of protein–RNA complexes. Rna, 2018, 24, 1183-1194.	3.5	84
10	ADMET Evaluation in Drug Discovery. Part 17: Development of Quantitative and Qualitative Prediction Models for Chemical-Induced Respiratory Toxicity. Molecular Pharmaceutics, 2017, 14, 2407-2421.	4.6	59
11	ADMET Evaluation in Drug Discovery. 18. Reliable Prediction of Chemical-Induced Urinary Tract Toxicity by Boosting Machine Learning Approaches. Molecular Pharmaceutics, 2017, 14, 3935-3953.	4.6	66
12	ADMET evaluation in drug discovery: 15. Accurate prediction of rat oral acute toxicity using relevance vector machine and consensus modeling. Journal of Cheminformatics, 2016, 8, 6.	6.1	102