Conrad Stork

List of Publications by Year
in descending order

18	449	932766 10	839053 18
papers	citations	h-index	g-index

18	18	18	586
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hit Dexter 2.0: Machine-Learning Models for the Prediction of Frequent Hitters. Journal of Chemical Information and Modeling, 2019, 59, 1030-1043.	2.5	70
2	FAME 3: Predicting the Sites of Metabolism in Synthetic Compounds and Natural Products for Phase 1 and Phase 2 Metabolic Enzymes. Journal of Chemical Information and Modeling, 2019, 59, 3400-3412.	2.5	60
3	GLORY: Generator of the Structures of Likely Cytochrome P450 Metabolites Based on Predicted Sites of Metabolism. Frontiers in Chemistry, 2019, 7, 402.	1.8	57
4	FAME 2: Simple and Effective Machine Learning Model of Cytochrome P450 Regioselectivity. Journal of Chemical Information and Modeling, 2017, 57, 1832-1846.	2.5	56
5	NERDD: a web portal providing access to in silico tools for drug discovery. Bioinformatics, 2020, 36, 1291-1292.	1.8	46
6	NP-Scout: Machine Learning Approach for the Quantification and Visualization of the Natural Product-Likeness of Small Molecules. Biomolecules, 2019, 9, 43.	1.8	43
7	Hit Dexter: A Machineâ€Learning Model for the Prediction of Frequent Hitters. ChemMedChem, 2018, 13, 564-571.	1.6	34
8	CYPlebrity: Machine learning models for the prediction of inhibitors of cytochrome P450 enzymes. Bioorganic and Medicinal Chemistry, 2021, 46, 116388.	1.4	16
9	Skin Doctor: Machine Learning Models for Skin Sensitization Prediction that Provide Estimates and Indicators of Prediction Reliability. International Journal of Molecular Sciences, 2019, 20, 4833.	1.8	15
10	Skin Doctor CP: Conformal Prediction of the Skin Sensitization Potential of Small Organic Molecules. Chemical Research in Toxicology, 2021, 34, 330-344.	1.7	11
11	PAIN(S) relievers for medicinal chemists: how computational methods can assist in hit evaluation. Future Medicinal Chemistry, 2018, 10, 1533-1535.	1.1	8
12	ALADDIN: Docking Approach Augmented by Machine Learning for Protein Structure Selection Yields Superior Virtual Screening Performance. Molecular Informatics, 2020, 39, e1900103.	1.4	8
13	Predicting the Skin Sensitization Potential of Small Molecules with Machine Learning Models Trained on Biologically Meaningful Descriptors. Pharmaceuticals, 2021, 14, 790.	1.7	7
14	Why Are Dithienyletheneâ€Linked Biscobaltocenes so Hard to Photoswitch?. ChemPhysChem, 2017, 18, 596-609.	1.0	5
15	CYPstrate: A Set of Machine Learning Models for the Accurate Classification of Cytochrome P450 Enzyme Substrates and Non-Substrates. Molecules, 2021, 26, 4678.	1.7	5
16	Computational Applications in Secondary Metabolite Discovery (CAiSMD): an online workshop. Journal of Cheminformatics, 2021, 13, 64.	2.8	3
17	Computational prediction of frequent hitters in target-based and cell-based assays. Artificial Intelligence in the Life Sciences, 2021, 1, 100007.	1.6	3
18	BonMOLiÃ¨re: Small-Sized Libraries of Readily Purchasable Compounds, Optimized to Produce Genuine Hits in Biological Screens across the Protein Space. International Journal of Molecular Sciences, 2021, 22, 7773.	1.8	2