Na Le Dang

List of Publications by Year in descending order

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933264 1058333 16 553 10 14 citations h-index g-index papers 17 17 17 1065 all docs docs citations times ranked citing authors

#	Article	IF	CITATIONS
1	Open Source Drug Discovery with the Malaria Box Compound Collection for Neglected Diseases and Beyond. PLoS Pathogens, 2016, 12, e1005763.	2.1	244
2	Modeling Reactivity to Biological Macromolecules with a Deep Multitask Network. ACS Central Science, 2016, 2, 529-537.	5.3	76
3	A simple model predicts UGT-mediated metabolism. Bioinformatics, 2016, 32, 3183-3189.	1.8	51
4	Computational Approach to Structural Alerts: Furans, Phenols, Nitroaromatics, and Thiophenes. Chemical Research in Toxicology, 2017, 30, 1046-1059.	1.7	32
5	Computationally Assessing the Bioactivation of Drugs by N-Dealkylation. Chemical Research in Toxicology, 2018, 31, 68-80.	1.7	30
6	The Metabolic Rainbow: Deep Learning Phase I Metabolism in Five Colors. Journal of Chemical Information and Modeling, 2020, 60, 1146-1164.	2.5	26
7	â€~Black Box' to â€~Conversational' Machine Learning: Ondansetron Reduces Risk of Hospital-Acquired Venous Thromboembolism. IEEE Journal of Biomedical and Health Informatics, 2021, 25, 2204-2214.	3.9	24
8	Learning a Local-Variable Model of Aromatic and Conjugated Systems. ACS Central Science, 2018, 4, 52-62.	5.3	18
9	XenoNet: Inference and Likelihood of Intermediate Metabolite Formation. Journal of Chemical Information and Modeling, 2020, 60, 3431-3449.	2.5	14
10	Metabolic Forest: Predicting the Diverse Structures of Drug Metabolites. Journal of Chemical Information and Modeling, 2020, 60, 4702-4716.	2.5	11
11	Modeling the Bioactivation and Subsequent Reactivity of Drugs. Chemical Research in Toxicology, 2021, 34, 584-600.	1.7	11
12	Deep learning long-range information in undirected graphs with wave networks. , 2019, , .		8
13	Deep Learning Coordinate-Free Quantum Chemistry. Journal of Physical Chemistry A, 2021, 125, 8978-8986.	1.1	5
14	Predictors of humoral response to SARS-CoV-2 mRNA vaccine BNT162b2 in patients receiving maintenance dialysis. Antimicrobial Stewardship & Healthcare Epidemiology, 2022, 2, .	0.2	2
15	SARS-CoV-2 Infection Risk Factors among Maintenance Hemodialysis Patients and Health Care Personnel In Outpatient Hemodialysis Centers. Kidney360, 2021, 2, 996-1001.	0.9	1
16	High Energy Channeling and Malleable Transition States: Molecular Dynamics Simulations and Free Energy Landscapes for the Thermal Unfolding of Protein U1A and 13 Mutants. Biomolecules, 2022, 12, 940.	1.8	0