Alexios Koutsoukas

List of Publications by Year
in descending order

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15 papers	677 citations	840776 11 h-index	996975 15 g-index
15 all docs	15 docs citations	15 times ranked	1059 citing authors

#	Article	IF	Citations
1	CLIFF: A component-based, machine-learned, intermolecular force field. Journal of Chemical Physics, 2021, 154, 184110.	3.0	18
2	Cartesian message passing neural networks for directional properties: Fast and transferable atomic multipoles. Journal of Chemical Physics, 2021, 154, 224103.	3.0	12
3	AP-Net: An atomic-pairwise neural network for smooth and transferable interaction potentials. Journal of Chemical Physics, 2020, 153, 044112.	3.0	41
4	Approaches for machine learning intermolecular interaction energies and application to energy components from symmetry adapted perturbation theory. Journal of Chemical Physics, 2020, 152, 074103.	3.0	25
5	Improving the prediction of organism-level toxicity through integration of chemical, protein target and cytotoxicity qHTS data. Toxicology Research, 2016, 5, 883-894.	2.1	10
6	Extending in silico mechanism-of-action analysis by annotating targets with pathways: application to cellular cytotoxicity readouts. Future Medicinal Chemistry, 2014, 6, 2029-2056.	2.3	19
7	How Diverse Are Diversity Assessment Methods? A Comparative Analysis and Benchmarking of Molecular Descriptor Space. Journal of Chemical Information and Modeling, 2014, 54, 230-242.	5.4	62
8	In Silico Target Predictions: Defining a Benchmarking Data Set and Comparison of Performance of the Multiclass NaÃ¯ve Bayes and Parzen-Rosenblatt Window. Journal of Chemical Information and Modeling, 2013, 53, 1957-1966.	5.4	131
9	Computerâ€aided (in silico) approaches in the modeâ€ofâ€action analysis and safety assessment of Ostarine and 4â€methylamphetamine. Human Psychopharmacology, 2013, 28, 365-378.	1.5	2
10	Experimental validation of in silico target predictions on synergistic protein targets. MedChemComm, 2013, 4, 278-288.	3.4	7
11	Chemogenomics Approaches to Rationalizing the Mode-of-Action of Traditional Chinese and Ayurvedic Medicines. Journal of Chemical Information and Modeling, 2013, 53, 661-673.	5.4	51
12	Diversity Selection of Compounds Based on â€˜Protein Affinity Fingerprintsâ€™ Improves Sampling of Bioactive Chemical Space. Chemical Biology and Drug Design, 2013, 82, 252-266.	3.2	19
13	Anti-cancer Drug Development: Computational Strategies to Identify and Target Proteins Involved in Cancer Metabolism. Current Pharmaceutical Design, 2013, 19, 532-577.	1.9	30
14	Linking Ayurveda and Western medicine by integrative analysis. Journal of Ayurveda and Integrative Medicine, 2013, 4, 117.	1.7	7
15	From in silico target prediction to multi-target drug design: Current databases, methods and applications. Journal of Proteomics, 2011, 74, 2554-2574.	2.4	243