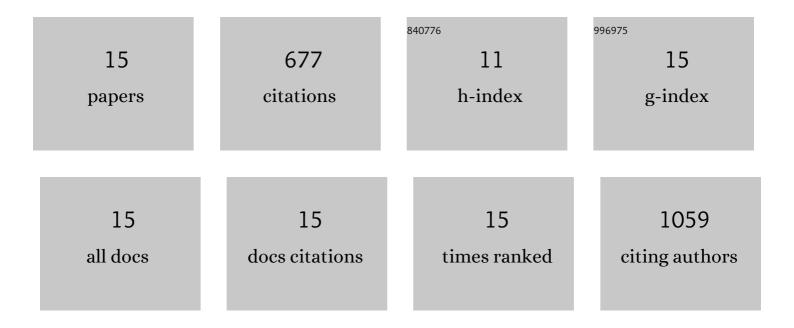
Alexios Koutsoukas

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	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
2	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
3	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
4	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
5	AP-Net: An atomic-pairwise neural network for smooth and transferable interaction potentials. Journal of Chemical Physics, 2020, 153, 044112.	3.0	41
6	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
7	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
8	Diversity Selection of Compounds Based on †Protein Affinity Fingerprints' Improves Sampling of <i>Bioactive</i> Chemical Space. Chemical Biology and Drug Design, 2013, 82, 252-266.	3.2	19
9	Extending <i>in silico</i> mechanism-of-action analysis by annotating targets with pathways: application to cellular cytotoxicity readouts. Future Medicinal Chemistry, 2014, 6, 2029-2056.	2.3	19
10	CLIFF: A component-based, machine-learned, intermolecular force field. Journal of Chemical Physics, 2021, 154, 184110.	3.0	18
11	Cartesian message passing neural networks for directional properties: Fast and transferable atomic multipoles. Journal of Chemical Physics, 2021, 154, 224103.	3.0	12
12	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
13	Experimental validation of <i>in silico</i> target predictions on synergistic protein targets. MedChemComm, 2013, 4, 278-288.	3.4	7
14	Linking Ayurveda and Western medicine by integrative analysis. Journal of Ayurveda and Integrative Medicine, 2013, 4, 117.	1.7	7
15	Computerâ€aided (<i>in silico</i>) approaches in the modeâ€ofâ€action analysis and safety assessment of Ostarine and 4â€methylamphetamine. Human Psychopharmacology, 2013, 28, 365-378.	1.5	2