# Alexios Koutsoukas

List of Publications by Year
in descending order

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

| # | 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 Naïve 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 *Bioactive* Chemical Space. Chemical Biology and Drug Design, 2013, 82, 252-266. | 3.2 | 19 |
| 9 | 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 |
| 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 *in silico* 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 | Computer-aided (*in silico*) approaches in the mode-of-action analysis and safety assessment of Ostarine and 4-methylamphetamine. Human Psychopharmacology, 2013, 28, 365-378. | 1.5 | 2 |