

Benedict W J Irwin

List of Publications by Year in descending order

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Version: 2024-02-01

11
papers

152
citations

1478505

6
h-index

1281871

11
g-index

14
all docs

14
docs citations

14
times ranked

193
citing authors

#	ARTICLE	IF	CITATIONS
1	Imputation of Assay Bioactivity Data Using Deep Learning. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 1197-1204.	5.4	48
2	Practical Applications of Deep Learning To Impute Heterogeneous Drug Discovery Data. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2848-2857.	5.4	35
3	Estimating Atomic Contributions to Hydration and Binding Using Free Energy Perturbation. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3218-3227.	5.3	20
4	Imputation versus prediction: applications in machine learning for drug discovery. <i>Future Drug Discovery</i> , 2020, 2, FDD38.	2.1	13
5	An Open Drug Discovery Competition: Experimental Validation of Predictive Models in a Series of Novel Antimalarials. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 16450-16463.	6.4	8
6	Large-Scale Study of Hydration Environments through Hydration Sites. <i>Journal of Physical Chemistry B</i> , 2019, 123, 4220-4229.	2.6	7
7	Deep imputation on large-scale drug discovery data. <i>Applied AI Letters</i> , 2021, 2, e31.	2.2	6
8	Functional movements of the GABA type A receptor. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16023-16031.	2.8	4
9	On the accuracy of one- and two-particle solvation entropies. <i>Journal of Chemical Physics</i> , 2017, 146, 194111.	3.0	3
10	Prediction of GABARAP interaction with the GABA type A receptor. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 1251-1264.	2.6	3
11	<sc>GABA</sc> receptor associated protein changes the electrostatic environment around the <sc>GABA</sc> type A receptor. <i>Proteins: Structure, Function and Bioinformatics</i> , 2022, 90, 476-484.	2.6	3