Lars Carlsson

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2151015/publications.pdf

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12	613	840776 11	1125743 13
papers	citations	h-index	g-index

13	13	13	1073
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Chemistry Development Kit (CDK) v2.0: atom typing, depiction, molecular formulas, and substructure searching. Journal of Cheminformatics, 2017, 9, 33.	6.1	275
2	Use of historic metabolic biotransformation data as a means of anticipating metabolic sites using MetaPrint2D and Bioclipse. BMC Bioinformatics, 2010, 11, 362.	2.6	66
3	The application of conformal prediction to the drug discovery process. Annals of Mathematics and Artificial Intelligence, 2015, 74, 117-132.	1.3	50
4	Ligand-Based Target Prediction with Signature Fingerprints. Journal of Chemical Information and Modeling, 2014, 54, 2647-2653.	5.4	40
5	Conformal Regression for Quantitative Structureâ€“Activity Relationship Modelingâ€”Quantifying Prediction Uncertainty. Journal of Chemical Information and Modeling, 2018, 58, 1132-1140.	5.4	35
6	Benchmarking Study of Parameter Variation When Using Signature Fingerprints Together with Support Vector Machines. Journal of Chemical Information and Modeling, 2014, 54, 3211-3217.	5.4	34
7	Integrated Decision Support for Assessing Chemical Liabilities. Journal of Chemical Information and Modeling, 2011, 51, 1840-1847.	5.4	31
8	Application of Bioactivity Profile-Based Fingerprints for Building Machine Learning Models. Journal of Chemical Information and Modeling, 2019, 59, 962-972.	5.4	24
9	Scaling Predictive Modeling in Drug Development with Cloud Computing. Journal of Chemical Information and Modeling, 2015, 55, 19-25.	5.4	12
10	Open Source Drug Discovery with Bioclipse. Current Topics in Medicinal Chemistry, 2012, 12, 1980-1986.	2.1	11
11	Improving machine learning in early drug discovery. Annals of Mathematics and Artificial Intelligence, 2017, 81, 155-166.	1.3	7
12	Current application of conformal prediction in drug discovery. Annals of Mathematics and Artificial Intelligence, 2017, 81, 145-154.	1.3	3