Nikolaus Stiefl

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8408068/publications.pdf

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14	384	933447 10	1058476 14
papers	citations	h-index	g-index

15	15	15	409
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Chemical Reactivity Prediction: Current Methods and Different Application Areas. Molecular Informatics, 2022, 41, .	2.5	6
2	GHOST: Adjusting the Decision Threshold to Handle Imbalanced Data in Machine Learning. Journal of Chemical Information and Modeling, 2021, 61, 2623-2640.	5.4	62
3	Ten simple rules to power drug discovery with data science. PLoS Computational Biology, 2020, 16, e1008126.	3.2	14
4	Evolution of Novartisâ€™ Small Molecule Screening Deck Design. Journal of Medicinal Chemistry, 2020, 63, 14425-14447.	6.4	31
5	Automated Identification of Chemical Series: Classifying like a Medicinal Chemist. Journal of Chemical Information and Modeling, 2020, 60, 2888-2902.	5.4	7
6	rdScaffoldNetwork: The Scaffold Network Implementation in RDKit. Journal of Chemical Information and Modeling, 2020, 60, 3331-3335.	5.4	23
7	Practical Aspects of Machine Learning for the Design-Synthesis-Purify-Assay Workflow. Chimia, 2018, 72, 648-649.	0.6	1
8	Chemical Topic Modeling: Exploring Molecular Data Sets Using a Common Text-Mining Approach. Journal of Chemical Information and Modeling, 2017, 57, 1816-1831.	5.4	12
9	Is that a scientific publication or an advertisement? Reproducibility, source code and data in the computational chemistry literature. Future Medicinal Chemistry, 2012, 4, 1885-1887.	2.3	5
10	A Knowledge-Based Weighting Approach to Ligand-Based Virtual Screening. Journal of Chemical Information and Modeling, 2006, 46, 587-596.	5.4	27
11	ErG:Â 2D Pharmacophore Descriptions for Scaffold Hopping. Journal of Chemical Information and Modeling, 2006, 46, 208-220.	5.4	100
12	Structure-Based Validation of the 3D-QSAR Technique MaP. Journal of Chemical Information and Modeling, 2005, 45, 739-749.	5.4	10
13	Evaluation of extended parameter sets for the 3D-QSAR technique MaP: implications for interpretability and model quality exemplified by antimalarially active naphthylisoquinoline alkaloids. Journal of Computer-Aided Molecular Design, 2003, 17, 347-365.	2.9	25
14	Mapping Property Distributions of Molecular Surfaces:â€‰Algorithm and Evaluation of a Novel 3D Quantitative Structureâˆ’Activity Relationship Technique. Journal of Medicinal Chemistry, 2003, 46, 1390-1407.	6.4	61