Nikolaus Stiefl

List of Publications by Year
in descending order

14 papers	384 citations	933447 10 h-index	1058476 14 g-index
15 all docs	15 docs citations	15 times ranked	409 citing authors

#	Article	IF	Citations
1	ErG: 2D Pharmacophore Descriptions for Scaffold Hopping. Journal of Chemical Information and Modeling, 2006, 46, 208-220.	5.4	100
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	Mapping Property Distributions of Molecular Surfaces:‰ Algorithm and Evaluation of a Novel 3D Quantitative Structure‑Activity Relationship Technique. Journal of Medicinal Chemistry, 2003, 46, 1390-1407.	6.4	61
4	Evolution of Novartis' Small Molecule Screening Deck Design. Journal of Medicinal Chemistry, 2020, 63, 14425-14447.	6.4	31
5	A Knowledge-Based Weighting Approach to Ligand-Based Virtual Screening. Journal of Chemical Information and Modeling, 2006, 46, 587-596.	5.4	27
6	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
7	rdScaffoldNetwork: The Scaffold Network Implementation in RDKit. Journal of Chemical Information and Modeling, 2020, 60, 3331-3335.	5.4	23
8	Ten simple rules to power drug discovery with data science. PLoS Computational Biology, 2020, 16, e1008126.	3.2	14
9	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
10	Structure-Based Validation of the 3D-QSAR Technique MaP. Journal of Chemical Information and Modeling, 2005, 45, 739-749.	5.4	10
11	Automated Identification of Chemical Series: Classifying like a Medicinal Chemist. Journal of Chemical Information and Modeling, 2020, 60, 2888-2902.	5.4	7
12	Chemical Reactivity Prediction: Current Methods and Different Application Areas. Molecular Informatics, 2022, 41, .	2.5	6
13	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
14	Practical Aspects of Machine Learning for the Design-Synthesis-Purify-Assay Workflow. Chimia, 2018, 72, 648-649.	0.6	1