Simon Cross

List of Publications by Year in descending order

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1477746 1473754 9 340 9 6 citations h-index g-index papers 10 10 10 611 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	FLAP: GRID Molecular Interaction Fields in Virtual Screening. Validation using the DUD Data Set. Journal of Chemical Information and Modeling, 2010, 50, 1442-1450.	2.5	94
2	GRID-Based Three-Dimensional Pharmacophores I: FLAPpharm, a Novel Approach for Pharmacophore Elucidation. Journal of Chemical Information and Modeling, 2012, 52, 2587-2598.	2.5	76
3	Molecular fields in drug discovery: getting old or reaching maturity?. Drug Discovery Today, 2010, 15, 23-32.	3.2	67
4	GRID-Based Three-Dimensional Pharmacophores II: PharmBench, a Benchmark Data Set for Evaluating Pharmacophore Elucidation Methods. Journal of Chemical Information and Modeling, 2012, 52, 2599-2608.	2.5	36
5	Molecular interaction fields in drug discovery: recent advances and future perspectives. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 594-613.	6.2	36
6	Grid-derived structure-based 3D pharmacophores and their performance compared to docking. Drug Discovery Today: Technologies, 2010, 7, e213-e219.	4.0	15
7	Playing with Opening and Closing of Heterocycles: Using the Cusmano-Ruccia Reaction to Develop a Novel Class of Oxadiazolothiazinones, Active as Calcium Channel Modulators and P-Glycoprotein Inhibitors. Molecules, 2014, 19, 16543-16572.	1.7	6
8	Combining machine learning and quantum mechanics yields more <scp>chemically aware</scp> molecular descriptors for medicinal chemistry applications. Journal of Computational Chemistry, 2021, 42, 2068-2078.	1.5	6
9	FragExplorer: GRID-Based Fragment Growing and Replacement. Journal of Chemical Information and Modeling, 2022, 62, 1224-1235.	2.5	4