A Geoffrey Skillman

List of Publications by Year
in descending order

13 papers	3,810 citations	759233 12 h-index	1125743 13 g-index
13 all docs	13 docs citations	13 times ranked	5175 citing authors

#	Article	IF	Citations
1	Conformer Generation with OMEGA: Algorithm and Validation Using High Quality Structures from the Protein Databank and Cambridge Structural Database. Journal of Chemical Information and Modeling, 2010, 50, 572-584.	5.4	1,302
2	DOCK 4.0: search strategies for automated molecular docking of flexible molecule databases. Journal of Computer-Aided Molecular Design, 2001, 15, 411-428.	2.9	1,022
3	Comparison of Shape-Matching and Docking as Virtual Screening Tools. Journal of Medicinal Chemistry, 2007, 50, 74-82.	6.4	826
4	Potent, Low-Molecular-Weight Non-Peptide Inhibitors of Malarial Aspartyl Protease Plasmepsin II. Journal of Medicinal Chemistry, 1999, 42, 1428-1440.	6.4	173
5	Structure-based design and combinatorial chemistry yield low nanomolar inhibitors of cathepsin D. Chemistry and Biology, 1997, 4, 297-307.	6.0	146
6	How to do an evaluation: pitfalls and traps. Journal of Computer-Aided Molecular Design, 2008, 22, 179-190.	2.9	126
7	Novel Cathepsin D Inhibitors Block the Formation of Hyperphosphorylated Tau Fragments in Hippocampus. Journal of Neurochemistry, 2000, 74, 1469-1477.	3.9	67
8	Design, docking, and evaluation of multiple libraries against multiple targets. Proteins: Structure, Function and Bioinformatics, 2001, 42, 296-318.	2.6	66
9	A novel mechanism for inhibition of HIV-1 reverse transcriptase. Bioorganic Chemistry, 2002, 30, 443-458.	4.1	27
10	SAMPL6 challenge results from $$pK_a$$ predictions based on a general Gaussian process model. Journal of Computer-Aided Molecular Design, 2018, 32, 1165-1177.	2.9	20
11	A rapid method for exploring the protein structure universe. Proteins: Structure, Function and Bioinformatics, 1999, 34, 317-332.	2.6	15
12	Efficient calculation of SAMPL4 hydration free energies using OMEGA, SZYBKI, QUACPAC, and Zap TK. Journal of Computer-Aided Molecular Design, 2014, 28, 289-298.	2.9	13
13	Mechanistic Insights into Passive Membrane Permeability of Drug-like Molecules from a Weighted Ensemble of Trajectories. Journal of Chemical Information and Modeling, 2022, 62, 1891-1904.	5.4	7