Ryan G Coleman

List of Publications by Year
in descending order

14 papers	3,475 citations	623574 14 h-index	1058333 14 g-index
14 all docs	14 docs citations	14 times ranked	6128 citing authors

#	Article	IF	Citations
1	ZINC: A Free Tool to Discover Chemistry for Biology. Journal of Chemical Information and Modeling, 2012, 52, 1757-1768.	2.5	1,985
2	Structure-based maximal affinity model predicts small-molecule druggability. Nature Biotechnology, 2007, 25, 71-75.	9.4	615
3	Ligand discovery from a dopamine D3 receptor homology model and crystal structure. Nature Chemical Biology, 2011, 7, 769-778.	3.9	285
4	Ligand Pose and Orientational Sampling in Molecular Docking. PLoS ONE, 2013, 8, e75992.	1.1	139
5	Incorporation of protein flexibility and conformational energy penalties in docking screens to improve ligand discovery. Nature Chemistry, 2014, 6, 575-583.	6.6	124
6	Travel Depth, a New Shape Descriptor for Macromolecules: Application to Ligand Binding. Journal of Molecular Biology, 2006, 362, 441-458.	2.0	78
7	Protein Pockets: Inventory, Shape, and Comparison. Journal of Chemical Information and Modeling, 2010, 50, 589-603.	2.5	67
8	Finding and Characterizing Tunnels in Macromolecules with Application to Ion Channels and Pores. Biophysical Journal, 2009, 96, 632-645.	0.2	43
9	An intuitive approach to measuring protein surface curvature. Proteins: Structure, Function and Bioinformatics, 2005, 61, 1068-1074.	1.5	30
10	Structure-Based Identification of Small Molecule Binding Sites Using a Free Energy Model. Journal of Chemical Information and Modeling, 2006, 46, 2631-2637.	2.5	29
11	Protonation of Excited State Pyrene-1-Carboxylate by Phosphate and Organic Acids in Aqueous Solution Studied by Fluorescence Spectroscopy. Biophysical Journal, 2006, 91, 3864-3871.	0.2	26
12	SAMPL4 & DOCK3.7: lessons for automated docking procedures. Journal of Computer-Aided Molecular Design, 2014, 28, 201-209.	1.3	20
13	Shape and evolution of thermostable protein structure. Proteins: Structure, Function and Bioinformatics, 2010, 78, 420-433.	1.5	17
14	Chemical informatics uncovers a new role for moexipril as a novel inhibitor of cAMP phosphodiesterase-4 (PDE4). Biochemical Pharmacology, 2013, 85, 1297-1305.	2.0	17