

Ryan G Coleman

List of Publications by Year in descending order

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