Aqeel Ahmed

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/11755821/publications.pdf

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13	893	777949 13	1255698 13
papers	citations	h-index	g-index

13	13	13	1354
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Updates to Binding MOAD (Mother of All Databases): Polypharmacology Tools and Their Utility in Drug Repurposing. Journal of Molecular Biology, 2019, 431, 2423-2433.	2.0	62
2	CSAR 2014: A Benchmark Exercise Using Unpublished Data from Pharma. Journal of Chemical Information and Modeling, 2016, 56, 1063-1077.	2.5	88
3	CSAR Benchmark Exercise 2013: Evaluation of Results from a Combined Computational Protein Design, Docking, and Scoring/Ranking Challenge. Journal of Chemical Information and Modeling, 2016, 56, 1022-1031.	2.5	49
4	Recent improvements to Binding MOAD: a resource for proteinâ€“ligand binding affinities and structures. Nucleic Acids Research, 2015, 43, D465-D469.	6.5	92
5	Consensus among multiple approaches as a reliability measure for flexible fitting into cryo-EM data. Journal of Structural Biology, 2013, 182, 67-77.	1.3	20
6	CSAR Data Set Release 2012: Ligands, Affinities, Complexes, and Docking Decoys. Journal of Chemical Information and Modeling, 2013, 53, 1842-1852.	2.5	95
7	NMSim Web Server: integrated approach for normal mode-based geometric simulations of biologically relevant conformational transitions in proteins. Nucleic Acids Research, 2012, 40, W310-W316.	6.5	79
8	Consensus among flexible fitting approaches improves the interpretation of cryo-EM data. Journal of Structural Biology, 2012, 177, 561-570.	1.3	38
9	A Normal Mode-Based Geometric Simulation Approach for Exploring Biologically Relevant Conformational Transitions in Proteins. Journal of Chemical Information and Modeling, 2011, 51, 1604-1622.	2.5	62
10	Excited states of ribosome translocation revealed through integrative molecular modeling. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 18943-18948.	3.3	89
11	Largeâ€scale comparison of protein essential dynamics from molecular dynamics simulations and coarseâ€grained normal mode analyses. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3341-3352.	1.5	44
12	Colchicine Glycorandomization Influences Cytotoxicity and Mechanism of Action. Journal of the American Chemical Society, 2006, 128, 14224-14225.	6.6	87
13	Multiscale modeling of macromolecular conformational changes combining concepts from rigidity and elastic network theory. Proteins: Structure, Function and Bioinformatics, 2006, 63, 1038-1051.	1.5	88