Nahren Manuel Mascarenhas

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Understanding protein domain-swapping using structure-based models of protein folding. Progress in Biophysics and Molecular Biology, 2017, 128, 113-120.	2.9	42
2	A five-residue motif for the design of domain swapping in proteins. Nature Communications, 2019, 10, 452.	12.8	37
3	An efficient tool for identifying inhibitors based on 3D-QSAR and docking using feature-shape pharmacophore of biologically active conformation – A case study with CDK2/CyclinA. European Journal of Medicinal Chemistry, 2008, 43, 2807-2818.	5.5	33
4	Hybrid Structure-Based Virtual Screening Protocol for the Identification of Novel BACE1 Inhibitors. Journal of Chemical Information and Modeling, 2009, 49, 647-657.	5.4	26
5	Cysteine-3 and cysteine-4 are essential for the thioredoxin-like oxidoreductase and antioxidant activities of Plasmodium falciparum macrophage migration inhibitory factor. Free Radical Biology and Medicine, 2011, 50, 1659-1668.	2.9	21
6	How maltose influences structural changes to bind to maltoseâ€binding protein: Results from umbrella sampling simulation. Proteins: Structure, Function and Bioinformatics, 2013, 81, 185-198.	2.6	19
7	Protein Domain-Swapping Can Be a Consequence of Functional Residues. Journal of Physical Chemistry B, 2016, 120, 6929-6938.	2.6	19
8	Why pyridine containing pyrido[2,3-d]pyrimidin-7-ones selectively inhibit CDK4 than CDK2: Insights from molecular dynamics simulation. Journal of Molecular Graphics and Modelling, 2010, 28, 695-706.	2.4	16
9	Combined Ligand and Structure Based Approaches for Narrowing on the Essential Physicochemical Characteristics for CDK4 Inhibition. Journal of Chemical Information and Modeling, 2008, 48, 1325-1336.	5.4	14
10	Intrinsic Disorder in a Well-Folded Globular Protein. Journal of Physical Chemistry B, 2018, 122, 1876-1884.	2.6	5
11	Are different stoichiometries feasible for complexes between lymphotoxin-alpha and tumor necrosis factor receptor 1?. BMC Structural Biology, 2012, 12, 8.	2.3	4
12	Structure dictates the mechanism of ligand recognition in the histidine and maltose binding proteins. Current Research in Structural Biology, 2020, 2, 180-190.	2.2	4
13	Deciphering the Structural Requirements of Nucleoside Bisubstrate Analogues for Inhibition of MbtA in Mycobacterium tuberculosis: A FBâ€QSAR Study and Combinatorial Library Generation for Identifying Potential Hits. Molecular Informatics, 2011, 30, 863-872.	2.5	2