Mohammad Hossein Karimi-Jafari

List of Publications by Year
in descending order

20	216	1162367 8	1125271 13
papers	citations	h-index	g-index

21	21	21	324
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Insights into the molecular interaction between two polyoxygenated cinnamoylcoumarin derivatives and human serum albumin. Physical Chemistry Chemical Physics, 2017, 19, 10099-10115.	1.3	36
2	Machine Learning and Network Analysis of Molecular Dynamics Trajectories Reveal Two Chains of Red/Ox-specific Residue Interactions in HumanÂProtein Disulfide Isomerase. Scientific Reports, 2017, 7, 3666.	1.6	33
3	iMM1865: A New Reconstruction of Mouse Genome-Scale Metabolic Model. Scientific Reports, 2020, 10, 6177.	1.6	21
4	Ensemble learning from ensemble docking: revisiting the optimum ensemble size problem. Scientific Reports, 2022, 12, 410.	1.6	16
5	Identification of a missense variant in CLDN2 in obstructive azoospermia. Journal of Human Genetics, 2019, 64, 1023-1032.	1.1	14
6	Integration and gene co-expression network analysis of scRNA-seq transcriptomes reveal heterogeneity and key functional genes in human spermatogenesis. Scientific Reports, 2021, 11, 19089.	1.6	12
7	Prediction of antimicrobial peptides toxicity based on their physico-chemical properties using machine learning techniques. BMC Bioinformatics, 2021, 22, 549.	1.2	12
8	Histidine substitution in the most flexible fragments of firefly luciferase modifies its thermal stability. Archives of Biochemistry and Biophysics, 2017, 629, 8-18.	1.4	10
9	Efficient construction of a diverse conformational library for amyloid-Î² as an intrinsically disordered protein. Journal of Molecular Graphics and Modelling, 2019, 88, 183-193.	1.3	9
10	Using the Semiempirical Quantum Mechanics in Improving the Molecular Docking: A Case Study with CDK2. Molecular Informatics, 2020, 39, e2000036.	1.4	9
11	ETâ€score: Improving Proteinâ€ligand Binding Affinity Prediction Based on Distanceâ€weighted Interatomic Contact Features Using Extremely Randomized Trees Algorithm. Molecular Informatics, 2021, 40, e2060084.	1.4	9
12	Hersintuzumab: A novel humanized anti-HER2 monoclonal antibody induces potent tumor growth inhibition. Investigational New Drugs, 2018, 36, 171-186.	1.2	8
13	Low-energy conformers of pamidronate and their intramolecular hydrogen bonds: a DFT and QTAIM study. Journal of Molecular Modeling, 2013, 19, 427-438.	0.8	5
14	Biological evaluation of 9-(1H-Indol-3-yl) xanthen-4-(9H)-ones derivatives as noncompetitive Î±-glucosidase inhibitors: kinetics and molecular mechanisms. Structural Chemistry, 2019, 30, 703-714.	1.0	5
15	Structural insights into the substrateâ€binding site of main protease for the structureâ€based COVIDâ€19 drug discovery. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1090-1101.	1.5	5
16	Red/ox states of human protein disulfide isomerase regulate binding affinity of 17 beta-estradiol. Archives of Biochemistry and Biophysics, 2017, 619, 35-44.	1.4	4
17	Electrostatically induced pKa shifts in oligopeptides: the upshot of neighboring side chains. Amino Acids, 2022, 54, 277.	1.2	4
18	Complexation of Sm3+ and pamidronate: A DFT study. Journal of Rare Earths, 2015, 33, 310-319.	2.5	2

#	Article	IF	Citations
19	Micro-solvation of a bisphosphonate group: an ab initio and effective fragment potential analysis. Structural Chemistry, 2017, 28, 1201-1210.	1.0	1
20	Binder design for targeting SARS-CoV-2 spike protein: An in silico perspective. Gene Reports, 2022, 26, 101452.	0.4	1