

Mohammad Hossein Karimi-Jafari

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

19
papers

101
citations

5
h-index

8
g-index

21
ext. papers

159
ext. citations

3.5
avg, IF

2.55
L-index

#	Paper	IF	Citations
19	Electrostatically induced pK shifts in oligopeptides: the upshot of neighboring side chains.. <i>Amino Acids</i> , 2022 , 54, 277	3.5	2
18	Ensemble learning from ensemble docking: revisiting the optimum ensemble size problem.. <i>Scientific Reports</i> , 2022 , 12, 410	4.9	2
17	Binder design for targeting SARS-CoV-2 spike protein: An in silico perspective. <i>Gene Reports</i> , 2022 , 26, 101452	1.4	1
16	Prediction of antimicrobial peptides toxicity based on their physico-chemical properties using machine learning techniques. <i>BMC Bioinformatics</i> , 2021 , 22, 549	3.6	3
15	ET-score: Improving Protein-ligand Binding Affinity Prediction Based on Distance-weighted Interatomic Contact Features Using Extremely Randomized Trees Algorithm. <i>Molecular Informatics</i> , 2021 , 40, e2060084	3.8	2
14	Integration and gene co-expression network analysis of scRNA-seq transcriptomes reveal heterogeneity and key functional genes in human spermatogenesis. <i>Scientific Reports</i> , 2021 , 11, 19089	4.9	1
13	Using the Semiempirical Quantum Mechanics in Improving the Molecular Docking: A Case Study with CDK2. <i>Molecular Informatics</i> , 2020 , 39, e2000036	3.8	4
12	iMM1865: A New Reconstruction of Mouse Genome-Scale Metabolic Model. <i>Scientific Reports</i> , 2020 , 10, 6177	4.9	6
11	Efficient construction of a diverse conformational library for amyloid- β s an intrinsically disordered protein. <i>Journal of Molecular Graphics and Modelling</i> , 2019 , 88, 183-193	2.8	3
10	Identification of a missense variant in CLDN2 in obstructive azoospermia. <i>Journal of Human Genetics</i> , 2019 , 64, 1023-1032	4.3	7
9	Biological evaluation of 9-(1H-Indol-3-yl) xanthen-4-(9H)-ones derivatives as noncompetitive Eglucosidase inhibitors: kinetics and molecular mechanisms. <i>Structural Chemistry</i> , 2019 , 30, 703-714	1.8	4
8	Hersintuzumab: A novel humanized anti-HER2 monoclonal antibody induces potent tumor growth inhibition. <i>Investigational New Drugs</i> , 2018 , 36, 171-186	4.3	5
7	Micro-solvation of a bisphosphonate group: an ab initio and effective fragment potential analysis. <i>Structural Chemistry</i> , 2017 , 28, 1201-1210	1.8	1
6	Machine Learning and Network Analysis of Molecular Dynamics Trajectories Reveal Two Chains of Red/Ox-specific Residue Interactions in Human β Protein Disulfide Isomerase. <i>Scientific Reports</i> , 2017 , 7, 3666	4.9	18
5	Insights into the molecular interaction between two polyoxygenated cinnamoylcoumarin derivatives and human serum albumin. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 10099-10115	3.6	27
4	Red/ox states of human protein disulfide isomerase regulate binding affinity of 17 beta-estradiol. <i>Archives of Biochemistry and Biophysics</i> , 2017 , 619, 35-44	4.1	3
3	Histidine substitution in the most flexible fragments of firefly luciferase modifies its thermal stability. <i>Archives of Biochemistry and Biophysics</i> , 2017 , 629, 8-18	4.1	4

- 2 Complexation of Sm³⁺ and pamidronate: A DFT study. *Journal of Rare Earths*, **2015**, 33, 310-319 3.7 2
- 1 Low-energy conformers of pamidronate and their intramolecular hydrogen bonds: a DFT and QTAIM study. *Journal of Molecular Modeling*, **2013**, 19, 427-38 2 5