Nadjib Melkemi

List of Publications by Year
in descending order

10	121	1684188 5	1372567 10
papers	citations	h-index	g-index

10	10	10	189
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Combined QSAR, molecular docking and molecular dynamics study on new Acetylcholinesterase and Butyrylcholinesterase inhibitors. Computational Biology and Chemistry, 2018, 74, 304-326.	2.3	68
2	DFT-based reactivity and combined QSAR, molecular docking of 1,2,4,5-Tetrazine derivatives as inhibitors of Pim-1 kinase. Heliyon, 2019, 5, e02451.	3.2	10
3	K-means clustering analysis, ADME/pharmacokinetic prediction, MEP, and molecular docking studies of potential cytotoxic agents. Structural Chemistry, 2021, 32, 2235-2249.	2.0	10
4	Structure-Property Relationships and Quantitative Structure-Activity Relationship Modeling of Detoxication Properties of Some 1,2-Dithiole-3-Thione Derivatives. Journal of Computational and Theoretical Nanoscience, 2014, 11, 801-806.	0.4	8
5	Structure Activity Relationship and Quantitative Structure-Activity Relationships Modeling of Antitrypanosomal Activities of Alkyldiamine Cryptolepine Derivatives. Journal of Computational and Theoretical Nanoscience, 2015, 12, 2421-2427.	0.4	7
6	Discovery of potential SARS-CoV 3CL protease inhibitors from approved antiviral drugs using: virtual screening, molecular docking, pharmacophore mapping evaluation and dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2021, , 1-18.	3.5	6
7	Molecular Geometry, Electronic Properties, MPO Methods and Structure Activity/Property Relationship Studies of 1,3,4-Thiadiazole Derivatives by Theoretical Calculations. Reviews in Theoretical Science, 2015, 3, 355-364.	0.5	5
8	Molecular docking/dynamic simulations, MEP, ADME-TOX-based analysis of xanthone derivatives as CHK1 inhibitors. Structural Chemistry, 2022, 33, 833-858.	2.0	4
9	In silico investigation by conceptual DFT and molecular docking of antitrypanosomal compounds for understanding cruzain inhibition. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650021.	1.8	2
10	Conformational Analysis and Physical-Chemistry Property Relationship for 22-Membered Macrolides. Asian Journal of Chemistry, 2013, 25, 4527-4531.	0.3	1