

Nadjib Melkemi

List of Publications by Year in descending order

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Version: 2024-02-01

10
papers

121
citations

1684188

5
h-index

1372567

10
g-index

10
all docs

10
docs citations

10
times ranked

189
citing authors

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