

Emilio L Angelina

List of Publications by Year in descending order

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Version: 2024-02-01

21
papers

363
citations

933447

10
h-index

794594

19
g-index

21
all docs

21
docs citations

21
times ranked

407
citing authors

#	ARTICLE	IF	CITATIONS
1	Evaluating the conformational space of the active site of D_2 dopamine receptor. Scope and limitations of the standard docking methods. <i>Journal of Computational Chemistry</i> , 2022, 43, 1298-1312.	3.3	2
2	Covalence and π -electron delocalization influence on hydrogen bonds in proton transfer process of <i>o</i> -hydroxy aryl Schiff bases: A combined NMR and QTAIM analysis. <i>Journal of Chemical Physics</i> , 2021, 155, 054307.	3.0	2
3	Design, synthesis, biological evaluation and molecular modelling of substituted pyrrolo[2,1-a]isoquinolinone derivatives: discovery of potent inhibitors of AChE and BChE. <i>New Journal of Chemistry</i> , 2021, 45, 8321-8334.	2.8	3
4	Hydroxynaphthalenecarboxamides and substituted piperazinypropandiols, two new series of BRAF inhibitors. A theoretical and experimental study. <i>Bioorganic Chemistry</i> , 2020, 103, 104145.	4.1	8
5	Conformational and electronic study of dopamine interacting with the D_2 dopamine receptor. <i>Journal of Computational Chemistry</i> , 2020, 41, 1898-1911.	3.3	9
6	Searching new structural scaffolds for BRAF inhibitors. An integrative study using theoretical and experimental techniques. <i>Bioorganic Chemistry</i> , 2019, 91, 103125.	4.1	9
7	Combining Charge Density Analysis with Machine Learning Tools To Investigate the Cruzain Inhibition Mechanism. <i>ACS Omega</i> , 2019, 4, 19582-19594.	3.5	13
8	Flap-site Fragment Restores Back Wild-type Behaviour in Resistant Form of HIV Protease. <i>Molecular Informatics</i> , 2018, 37, 1800053.	2.5	2
9	New small-size peptides modulators of the exosite of BACE1 obtained from a structure-based design. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017, 35, 413-426.	3.5	17
10	The electronic density obtained from a QTAIM analysis used as molecular descriptor. A study performed in a new series of DHFR inhibitors. <i>Journal of Molecular Structure</i> , 2017, 1134, 464-474.	3.6	16
11	Tetrahydroisoquinolines functionalized with carbamates as selective ligands of D_2 dopamine receptor. <i>Journal of Molecular Modeling</i> , 2017, 23, 273.	1.8	9
12	An integrative study to identify novel scaffolds for sphingosine kinase 1 inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2017, 139, 461-481.	5.5	33
13	Halogen bonding in biological context: a computational study of D_2 dopamine receptor. <i>Journal of Physical Organic Chemistry</i> , 2016, 29, 645-655.	1.9	21
14	Pentameric models as alternative molecular targets for the design of new antiaggregant agents. <i>Current Protein and Peptide Science</i> , 2016, 17, 156-168.	1.4	12
15	α -Chlorotyramine Acting as Ligand of the D_2 Dopamine Receptor. <i>Molecular Modeling, Synthesis and D_2 Receptor Affinity</i> . <i>Molecular Informatics</i> , 2015, 34, 28-43.	2.5	10
16	Non-covalent interactions in receptor-ligand complexes. A study based on the electron charge density. <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 128-134.	1.9	29
17	Molecular Modeling Study of Dihydrofolate Reductase Inhibitors. <i>Molecular Dynamics Simulations, Quantum Mechanical Calculations, and Experimental Corroboration</i> . <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2018-2032.	5.4	56
18	2,3,9- and 2,3,11-Trisubstituted tetrahydroprotoberberines as D_2 dopaminergic ligands. <i>European Journal of Medicinal Chemistry</i> , 2013, 68, 150-166.	5.5	37

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19	On the strength of the halogen bonds: Mutual penetration, atomic quadrupole moment and Laplacian distribution of the charge density analyses. <i>Computational and Theoretical Chemistry</i> , 2012, 998, 164-172.	2.5	24
20	Searching the "Biologically Relevant" Conformation of Dopamine: A Computational Approach. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 99-112.	5.4	48
21	Study of polyphenols from <i>Caesalpinia paraguariensis</i> as α -glucosidase inhibitors: kinetics and structure-activity relationship. <i>New Journal of Chemistry</i> , 0, , .	2.8	3