Rodrigo Aguayo-Ortiz

List of Publications by Year
in descending order

46	708	567144 15	610775 24
papers	citations	h-index	g-index

48	48	48	1057
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular basis for benzimidazole resistance from a novel Î²-tubulin binding site model. Journal of Molecular Graphics and Modelling, 2013, 45, 26-37.	1.3	61
2	Characterizing the structural ensemble of Î³-secretase using a multiscale molecular dynamics approach. Chemical Science, 2017, 8, 5576-5584.	3.7	55
3	Towards the identification of the binding site of benzimidazoles to Î²-tubulin of Trichinella spiralis: Insights from computational and experimental data. Journal of Molecular Graphics and Modelling, 2013, 41, 12-19.	1.3	54
4	Synthesis, hypoglycemic activity and molecular modeling studies of pyrazole-3-carbohydrazides designed by a CoMFA model. European Journal of Medicinal Chemistry, 2013, 69, 10-21.	2.6	40
5	Resveratrol-salicylate derivatives as selective DNMT3 inhibitors and anticancer agents. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 695-703.	2.5	40
6	Linking Biochemical and Structural States of SERCA: Achievements, Challenges, and New Opportunities. International Journal of Molecular Sciences, 2020, 21, 4146.	1.8	36
7	Dwarf open reading frame (DWORF) is a direct activator of the sarcoplasmic reticulum calcium pump SERCA. ELife, 2021, 10, .	2.8	31
8	Curcumin alters the cytoskeleton and microtubule organization on trophozoites of Giardia lamblia. Acta Tropica, 2017, 172, 113-121.	0.9	30
9	Anti-inflammatory and antioxidant properties of a novel resveratrolâ€“salicylate hybrid analog. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 1411-1415.	1.0	27
10	Synthesis, antiprotozoal activity, and chemoinformatic analysis of 2-(methylthio)-1H-benzimidazole-5-carboxamide derivatives: Identification of new selective giardicidal and trichomonicidal compounds. European Journal of Medicinal Chemistry, 2017, 137, 211-220.	2.6	23
11	Identification and Characterization of Novel Receptor-Interacting Serine/Threonineâ€Protein Kinase 2 Inhibitors Using Structural Similarity Analysis. Journal of Pharmacology and Experimental Therapeutics, 2018, 365, 354-367.	1.3	22
12	Untying the knot of transcription factor druggability: Molecular modeling study of FOXM1 inhibitors. Journal of Molecular Graphics and Modelling, 2018, 80, 197-210.	1.3	21
13	Influence of membrane lipid composition on the structure and activity of Î³-secretase. Physical Chemistry Chemical Physics, 2018, 20, 27294-27304.	1.3	20
14	Insights into the structure and inhibition ofGiardia intestinalisarginine deiminase: homology modeling, docking, and molecular dynamics studies. Journal of Biomolecular Structure and Dynamics, 2016, 34, 732-748.	2.0	16
15	Structureâ€based approaches for the design of benzimidazoleâ€2â€carbamate derivatives as tubulin polymerization inhibitors. Chemical Biology and Drug Design, 2017, 90, 40-51.	1.5	16
16	Toward the Characterization of DAPT Interactions with Î³â€Secretase. ChemMedChem, 2019, 14, 1005-1010.	1.6	16
17	Effects of the Protonation State of Titratable Residues and the Presence of Water Molecules on Nocodazole Binding to Î²â€Tubulin. ChemMedChem, 2018, 13, 20-24.	1.6	15
18	Simulating the Î³-secretase enzyme: Recent advances and future directions. Biochimie, 2018, 147, 130-135.	1.3	14

#	Article	IF	Citations
19	Synthesis of a poly(ester) dendritic Î²-cyclodextrin derivative by â€œclickâ€•chemistry: Combining the best of two worlds for complexation enhancement. Carbohydrate Polymers, 2018, 184, 20-29.	5.1	14
20	Design and synthesis of resveratrolâ€“salicylate hybrid derivatives as CYP1A1 inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 30, 884-895.	2.5	13
21	Progress in the Visualization and Mining of Chemical and Target Spaces. Molecular Informatics, 2013, 32, 942-953.	1.4	10
22	Chemoinformatic characterization of activity and selectivity switches of antiprotozoal compounds. Future Medicinal Chemistry, 2014, 6, 281-294.	1.1	10
23	Effects of Mutating Trp42 Residue on Î³D-Crystallin Stability. Journal of Chemical Information and Modeling, 2020, 60, 777-785.	2.5	10
24	A multiscale approach for bridging the gap between potency, efficacy, and safety of small molecules directed at membrane proteins. Scientific Reports, 2021, 11, 16580.	1.6	10
25	Dynamics-Driven Allostery Underlies Ca2+-Mediated Release of SERCA Inhibition by Phospholamban. Biophysical Journal, 2020, 119, 1917-1926.	0.2	10
26	Overview of Computer-Aided Drug Design for Epigenetic Targets. , 2016, , 21-52.		9
27	Thermodynamic Stability of Human Î³D-Crystallin Mutants Using Alchemical Free-Energy Calculations. Journal of Physical Chemistry B, 2019, 123, 5671-5677.	1.2	8
28	APH-1A Component of Î³-Secretase Forms an Internal Water and Ion-Containing Cavity. ACS Chemical Neuroscience, 2019, 10, 2931-2938.	1.7	7
29	Synthesis, in vitro, in silico and in vivo hypoglycemic and lipid-lowering effects of 4-benzyloxy-5-benzylidene-1,3-thiazolidine-2,4-diones mediated by dual PPAR Î±/Î³ modulation. Bioorganic and Medicinal Chemistry Letters, 2022, 70, 128804.	1.0	7
30	Atomistic Structure and Dynamics of the Ca2+-ATPase Bound to Phosphorylated Phospholamban. International Journal of Molecular Sciences, 2020, 21, 7261.	1.8	6
31	Disruption of TFIIH activities generates a stress gene expression response and reveals possible new targets against cancer. Open Biology, 2020, 10, 200050.	1.5	5
32	Characterizing the Chemical Space of Î³-Secretase Inhibitors and Modulators. ACS Chemical Neuroscience, 2021, 12, 2765-2775.	1.7	5
33	In Silico Characterization of Masitinib Interaction with SARSâ€CoVâ€2 Main Protease. ChemMedChem, 2021, 16, 2339-2344.	1.6	5
34	Identification and In Silico Characterization of Novel Helicobacter pylori Glucose-6-Phosphate Dehydrogenase Inhibitors. Molecules, 2021, 26, 4955.	1.7	5
35	Kinetic and Molecular Docking Studies to Determine the Effect of Inhibitors on the Activity and Structure of Fused G6PD::6PGL Protein from Trichomonas vaginalis. Molecules, 2022, 27, 1174.	1.7	5
36	Unveiling the Possible Oryzalin-Binding Site in the Î±-Tubulin of Toxoplasma gondii. ACS Omega, 2022, 7, 18434-18442.	1.6	5

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37	Quantifying correlations between mutational sites in the catalytic subunit of Î³-secretase. Journal of Molecular Graphics and Modelling, 2019, 88, 221-227.	1.3	4
38	Design, Synthesis and Evaluation of 2,4â€Diaminoquinazoline Derivatives as Potential Tubulin Polymerization Inhibitors. ChemMedChem, 2020, 15, 1802-1812.	1.6	4
39	Insights into the binding of morin to human Î³D-crystallin. Biophysical Chemistry, 2022, 282, 106750.	1.5	4
40	Homologous cardiac calcium pump regulators phospholamban and sarcolipin adopt distinct oligomeric states in the membrane. Computational and Structural Biotechnology Journal, 2022, 20, 380-384.	1.9	4
41	Conserved Luminal C-Terminal Domain Dynamically Controls Interdomain Communication in Sarcolipin. Journal of Chemical Information and Modeling, 2020, 60, 3985-3991.	2.5	3
42	A hallmark of phospholamban functional divergence is located in the N-terminal phosphorylation domain. Computational and Structural Biotechnology Journal, 2020, 18, 705-713.	1.9	3
43	Primitive Phospholamban- and Sarcolipin-like Peptides Inhibit the Sarcoplasmic Reticulum Calcium Pump SERCA. Biochemistry, 2022, 61, 1419-1430.	1.2	2
44	Generation of Amyloidâ€Î² Peptides by Î³â€Secretase. Israel Journal of Chemistry, 2017, 57, 574-585.	1.0	1
45	Evaluation of New Benzimidazole Derivatives as Cysticidal Agents: <i>In Vitro</i>, <i>in Vivo</i> and Docking Studies. Chemical and Pharmaceutical Bulletin, 2019, 67, 1293-1300.	0.6	1
46	Total syntheses and antiproliferative activities of prenostodione and its analogues. Organic and Biomolecular Chemistry, 2021, 19, 8272-8280.	1.5	0