Rodrigo Aguayo-Ortiz

List of Publications by Year
in descending order

46	708	566801 15	610482 24
papers	citations	h-index	g-index

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

#	Article	IF	Citations
1	Insights into the binding of morin to human Î³D-crystallin. Biophysical Chemistry, 2022, 282, 106750.	1.5	4
2	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
3	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
4	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
5	Unveiling the Possible Oryzalin-Binding Site in the Î±-Tubulin of Toxoplasma gondii. ACS Omega, 2022, 7, 18434-18442.	1.6	5
6	Primitive Phospholamban- and Sarcolipin-like Peptides Inhibit the Sarcoplasmic Reticulum Calcium Pump SERCA. Biochemistry, 2022, 61, 1419-1430.	1.2	2
7	Dwarf open reading frame (DWORF) is a direct activator of the sarcoplasmic reticulum calcium pump SERCA. ELife, 2021, 10, .	2.8	31
8	Characterizing the Chemical Space of Î³-Secretase Inhibitors and Modulators. ACS Chemical Neuroscience, 2021, 12, 2765-2775.	1.7	5
9	In Silico Characterization of Masitinib Interaction with SARSâ€CoVâ€2 Main Protease. ChemMedChem, 2021, 16, 2339-2344.	1.6	5
10	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
11	Identification and In Silico Characterization of Novel Helicobacter pylori Glucose-6-Phosphate Dehydrogenase Inhibitors. Molecules, 2021, 26, 4955.	1.7	5
12	Total syntheses and antiproliferative activities of prenostodione and its analogues. Organic and Biomolecular Chemistry, 2021, 19, 8272-8280.	1.5	0
13	Effects of Mutating Trp42 Residue on Î³D-Crystallin Stability. Journal of Chemical Information and Modeling, 2020, 60, 777-785.	2.5	10
14	Atomistic Structure and Dynamics of the Ca2+-ATPase Bound to Phosphorylated Phospholamban. International Journal of Molecular Sciences, 2020, 21, 7261.	1.8	6
15	Conserved Luminal C-Terminal Domain Dynamically Controls Interdomain Communication in Sarcolipin. Journal of Chemical Information and Modeling, 2020, 60, 3985-3991.	2.5	3
16	Design, Synthesis and Evaluation of 2,4â€Ðiaminoquinazoline Derivatives as Potential Tubulin Polymerization Inhibitors. ChemMedChem, 2020, 15, 1802-1812.	1.6	4
17	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
18	Linking Biochemical and Structural States of SERCA: Achievements, Challenges, and New Opportunities. International Journal of Molecular Sciences, 2020, 21, 4146.	1.8	36

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19	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
20	Dynamics-Driven Allostery Underlies Ca2+-Mediated Release of SERCA Inhibition by Phospholamban. Biophysical Journal, 2020, 119, 1917-1926.	0.2	10
21	Thermodynamic Stability of Human Î³D-Crystallin Mutants Using Alchemical Free-Energy Calculations. Journal of Physical Chemistry B, 2019, 123, 5671-5677.	1.2	8
22	Toward the Characterization of DAPT Interactions with Î³â€Secretase. ChemMedChem, 2019, 14, 1005-1010.	1.6	16
23	APH-1A Component of Î³-Secretase Forms an Internal Water and Ion-Containing Cavity. ACS Chemical Neuroscience, 2019, 10, 2931-2938.	1.7	7
24	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
25	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
26	Simulating the Î³-secretase enzyme: Recent advances and future directions. Biochimie, 2018, 147, 130-135.	1.3	14
27	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
28	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
29	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
30	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
31	Influence of membrane lipid composition on the structure and activity of Î³-secretase. Physical Chemistry Chemical Physics, 2018, 20, 27294-27304.	1.3	20
32	Curcumin alters the cytoskeleton and microtubule organization on trophozoites of Giardia lamblia. Acta Tropica, 2017, 172, 113-121.	0.9	30
33	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
34	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
35	Generation of Amyloidâ€Î² Peptides by Î³â€Secretase. Israel Journal of Chemistry, 2017, 57, 574-585.	1.0	1
36	Characterizing the structural ensemble of Î³-secretase using a multiscale molecular dynamics approach. Chemical Science, 2017, 8, 5576-5584.	3.7	55

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37	Overview of Computer-Aided Drug Design for Epigenetic Targets. , 2016, , 21-52.		9
38	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
39	Anti-inflammatory and antioxidant properties of a novel resveratrolâ€“salicylate hybrid analog. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 1411-1415.	1.0	27
40	Resveratrol-salicylate derivatives as selective DNMT3 inhibitors and anticancer agents. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 695-703.	2.5	40
41	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
42	Chemoinformatic characterization of activity and selectivity switches of antiprotozoal compounds. Future Medicinal Chemistry, 2014, 6, 281-294.	1.1	10
43	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
44	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
45	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
46	Progress in the Visualization and Mining of Chemical and Target Spaces. Molecular Informatics, 2013, 32, 942-953.	1.4	10