Ernesto R Caffarena

List of Publications by Year in Descending Order

64 papers	986 citations	17 h-index	29 g-index
75 ext. papers	1,181 ext. citations	3.6 avg, IF	4.39 L-index

#	Paper	IF	Citations
64	investigation of riboswitches in fungi: structural and dynamical insights into TPP riboswitches in .. *RNA Biology*, **2022**, 1-14	4.8	
63	pH and non-covalent ligand binding modulate Zika virus NS2B/NS3 protease binding site residues: Discoveries from MD and constant pH MD simulations. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-14	3.6	1
62	How does Histidine102 affect the binding of modulators to GABA receptors? molecular insights from experiments. *Physical Chemistry Chemical Physics*, **2021**, 23, 3993-4006	3.6	0
61	Insights into the Mechanism of Ethionamide Resistance in Mycobacterium tuberculosis through an in silico Structural Evaluation of EthA and Mutants Identified in Clinical Isolates. *Catalysts*, **2020**, 10, 543	4	3
60	Structural insights into NS5B protein of novel equine hepaciviruses and pegiviruses complexed with polymerase inhibitors. *Virus Research*, **2020**, 278, 197867	6.4	3
59	The rare lncRNA GOLLD is widespread and structurally conserved among tRNA arrays. *RNA Biology*, **2020**, 17, 1001-1008	4.8	0
58	Identification of Novel and Recurrent Variants in a Series of Brazilian Patients with Cartilage-Hair Hypoplasia: McKusick Syndrome. *Molecular Syndromology*, **2020**, 10, 255-263	1.5	2
57	Guidelines To Predict Binding Poses of Antibody-Integrin Complexes. *ACS Omega*, **2020**, 5, 16379-16385	3.9	1
56	Shared Binding Mode of Perrottetinene and Tetrahydrocannabinol Diastereomers inside the CB1 Receptor May Incentivize Novel Medicinal Drug Design: Findings from an Assay. *ACS Chemical Neuroscience*, **2020**, 11, 4289-4300	5.7	0
55	Studying effects of different protonation states of His11 and His102 in ribose-5-phosphate isomerase of : an example of cooperative behavior. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 2047-2056	3.6	4
54	and BCG Moreau Fumarate Reductase Operons Produce Different Polypeptides That May Be Related to Non-canonical Functions. *Frontiers in Microbiology*, **2020**, 11, 624121	5.7	2
53	Integrating Molecular Docking and Molecular Dynamics Simulations. *Methods in Molecular Biology*, **2019**, 2053, 13-34	1.4	19
52	Benzimidazole inhibitors of the major cysteine protease of. *Future Medicinal Chemistry*, **2019**, 11, 1537-1551	4.1	5
51	In silico analysis of the V66M variant of human BDNF in psychiatric disorders: An approach to precision medicine. *PLoS ONE*, **2019**, 14, e0215508	3.7	13
50	Unraveling RNA dynamical behavior of TPP riboswitches: a comparison between Escherichia coli and Arabidopsis thaliana. *Scientific Reports*, **2019**, 9, 4197	4.9	12
49	The role of hydrophobicity in the cold denaturation of proteins under high pressure: A study on apomyoglobin. *Journal of Chemical Physics*, **2019**, 150, 075102	3.9	5
48	Effects of the Q80K Polymorphism on the Physicochemical Properties of Hepatitis C Virus Subtype 1a NS3 Protease. *Viruses*, **2019**, 11,	6.2	1

47	Understanding Structure-Activity Relationships for Trypanosomal Cysteine Protease Inhibitors by Simulations and Free Energy Calculations. *Journal of Chemical Information and Modeling*, **2019**, 59, 137-148	6.1	14
46	Thiophenacetamide as a potential modulator to NF-B: structure and dynamics study using and molecular biology assays. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 4395-4406	3.6	3
45	Pressure effect on micellization of non-ionic surfactant Triton X-100. *Journal of Chemical Physics*, **2018**, 148, 074901	3.9	3
44	Antitumor Effect of Pomolic Acid in Acute Myeloid Leukemia Cells Involves Cell Death, Decreased Cell Growth and Topoisomerases Inhibition. *Anti-Cancer Agents in Medicinal Chemistry*, **2018**, 18, 1457-1468	2.2	0
43	Genomic and structural features of the yellow fever virus from the 2016-2017 Brazilian outbreak. *Journal of General Virology*, **2018**, 99, 536-548	4.9	30
42	Structural insights into leishmanolysins encoded on chromosome 10 of Leishmania (Viannia) braziliensis. *Memorias Do Instituto Oswaldo Cruz*, **2017**, 112, 617-625	2.6	4
41	Using RNA Sequence and Structure for the Prediction of Riboswitch Aptamer: A Comprehensive Review of Available Software and Tools. *Frontiers in Genetics*, **2017**, 8, 231	4.5	22
40	Essential dynamics of the cold denaturation: pressure and temperature effects in yeast frataxin. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 125-136	4.2	9
39	Evaluation of 7-arylaminopyrazolo[1,5-a]pyrimidines as anti-Plasmodium falciparum, antimalarial, and Pf-dihydroorotate dehydrogenase inhibitors. *European Journal of Medicinal Chemistry*, **2017**, 126, 72-83	6.8	43
38	Boosting Docking-Based Virtual Screening with Deep Learning. *Journal of Chemical Information and Modeling*, **2016**, 56, 2495-2506	6.1	175
37	Caracterizao do envelhecimento populacional no municpio do Rio de Janeiro: contribuies para polticas pblicas sustentveis. *Cadernos Saude Coletiva*, **2016**, 24, 63-69	0.3	5
36	Exploring the unbinding of Leishmania (L.) amazonensis CPB derived-epitopes from H2 MHC class I proteins. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 473-87	4.2	10
35	Structural and dynamic insights into the C-terminal extension of cysteine proteinase B from Leishmania amazonensis. *Journal of Molecular Graphics and Modelling*, **2016**, 70, 30-39	2.8	2
34	Gedunin Binds to Myeloid Differentiation Protein 2 and Impairs Lipopolysaccharide-Induced Toll-Like Receptor 4 Signaling in Macrophages. *Molecular Pharmacology*, **2015**, 88, 949-61	4.3	11
33	Computational drug design strategies applied to the modelling of human immunodeficiency virus-1 reverse transcriptase inhibitors. *Memorias Do Instituto Oswaldo Cruz*, **2015**, 110, 847-64	2.6	17
32	Epoxy-apachone has in vitro and in vivo anti-leishmania (Leishmania) amazonensis effects and inhibits serine proteinase activity in this parasite. *Antimicrobial Agents and Chemotherapy*, **2015**, 59, 1910-8	5.9	24
31	In Silico Identification of Novel APRIL Peptide Antagonists and Binding Insights by Molecular Modeling and Immunosorbent Assays. *Protein and Peptide Letters*, **2015**, 22, 432-42	1.9	1
30	Dynamic identification of H2 epitopes from Leishmania (Leishmania) amazonensis cysteine proteinase B with potential immune activity during murine infection. *Journal of Molecular Recognition*, **2014**, 27, 98-105	2.6	11

29	Structural and molecular modeling features of P2X receptors. *International Journal of Molecular Sciences*, **2014**, 15, 4531-49	6.3	15
28	Megazol and its bioisostere 4H-1,2,4-triazole: comparing the trypanocidal, cytotoxic and genotoxic activities and their in vitro and in silico interactions with the Trypanosoma brucei nitroreductase enzyme. *Memorias Do Instituto Oswaldo Cruz*, **2014**, 109, 315-23	2.6	13
27	Naturally occurring genetic variants of human caspase-1 differ considerably in structure and the ability to activate interleukin-1 *Human Mutation*, **2013**, 34, 122-31	4.7	28
26	Toll-like receptor 1 N248S single-nucleotide polymorphism is associated with leprosy risk and regulates immune activation during mycobacterial infection. *Journal of Infectious Diseases*, **2013**, 208, 120-9	7	38
25	PLAUSIBLE BINDING MODE OF THE ACTIVE 41 ANTAGONIST, MK-0617, DETERMINED BY DOCKING AND FREE ENERGY CALCULATIONS. *Journal of Theoretical and Computational Chemistry*, **2013**, 12, 1250108	1.8	6
24	Molecular interactions of c-ABL mutants in complex with imatinib/nilotinib: a computational study using linear interaction energy (LIE) calculations. *Journal of Molecular Modeling*, **2012**, 18, 4333-41	2	5
23	Computational modeling of the bHLH domain of the transcription factor TWIST1 and R118C, S144R and K145E mutants. *BMC Bioinformatics*, **2012**, 13, 184	3.6	18
22	Structure-based functional inference of hypothetical proteins from Mycoplasma hyopneumoniae. *Journal of Molecular Modeling*, **2012**, 18, 1917-25	2	12
21	In silico predicted epitopes from the COOH-terminal extension of cysteine proteinase B inducing distinct immune responses during Leishmania (Leishmania) amazonensis experimental murine infection. *BMC Immunology*, **2011**, 12, 44	3.7	21
20	Analysis of 4 1integrin specific antagonists binding modes: structural insights by molecular docking, molecular dynamics and linear interaction energy method for free energy calculations. *Journal of the Brazilian Chemical Society*, **2010**, 21, 546-555	1.5	5
19	New parameterization approaches of the LIE method to improve free energy calculations of PlmII-Inhibitors complexes. *Journal of Computational Chemistry*, **2010**, 31, 2723-34	3.5	14
18	Dissociation of molecular aggregates under high hydrostatic pressure: the influence of water structure on Benzene cluster solubility. *Journal of the Brazilian Chemical Society*, **2009**, 20, 1227-1234	1.5	7
17	Water behavior in the neighborhood of hydrophilic and hydrophobic membranes: Lessons from molecular dynamics simulations. *Physica A: Statistical Mechanics and Its Applications*, **2009**, 388, 4551-4559	2.3	8
16	Synthesis, antimalarial evaluation and molecular modeling studies of hydroxyethylpiperazines, potential aspartyl protease inhibitors, part 2. *European Journal of Medicinal Chemistry*, **2009**, 44, 3816-20	6.8	24
15	Predictions suggesting a participation of beta-sheet configuration in the M2 domain of the P2X(7) receptor: a novel conformation?. *Biophysical Journal*, **2009**, 96, 951-63	2.9	5
14	Studies of molecular docking between fibroblast growth factor and heparin using generalized simulated annealing. *International Journal of Quantum Chemistry*, **2008**, 108, 2608-2614	2.1	8
13	Molecular docking study and development of an empirical binding free energy model for phosphodiesterase 4 inhibitors. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 6001-11	3.4	14
12	Conformational and dynamical properties of the niruriside in aqueous solution: a molecular dynamics approach. *Computational and Theoretical Chemistry*, **2005**, 714, 189-197		2

11	Elastic properties, Young's modulus determination and structural stability of the tropocollagen molecule: a computational study by steered molecular dynamics. *Journal of Biomechanics*, **2005**, 38, 1527-33	2.9	118
10	On the hydrogen bond structure of water at different densities. *Physica A: Statistical Mechanics and Its Applications*, **2004**, 342, 34-39	3.3	19
9	Stochastic molecular dynamics of peanut lectin PNA complex with T-antigen disaccharide. *Journal of Molecular Graphics and Modelling*, **2002**, 21, 227-40	2.8	7
8	Hydration of T-antigen Gal beta(1-3)GalNAc and the isomer Gal beta(1-3)GlcNAc by molecular dynamics simulations. *Journal of Molecular Graphics and Modelling*, **2000**, 18, 119-25	2.8	4
7	Hydration of glucose in the rubbery and glassy states studied by molecular dynamics simulation. *Carbohydrate Research*, **1999**, 315, 63-69	2.9	36
6	Computer simulation of the cyclodextrin□phenylalanine complex. *Carbohydrate Research*, **1998**, 310, 253-259	2.9	16
5	Hydrogen Bonding of Carboxylic Acids in Aqueous Solutions□UV Spectroscopy, Viscosity, and Molecular Simulation of Acetic Acid. *Journal of Solution Chemistry*, **1998**, 27, 935-948	1.8	27
4	Hydration properties of xylitol: computer simulation. *International Journal of Biological Macromolecules*, **1998**, 23, 149-55	7.9	8
3	Glass transition in aqueous solutions of glucose. Molecular dynamics simulation. *Carbohydrate Research*, **1997**, 300, 51-57	2.9	35
2	Crystal, melted and glassy states of glucose. A molecular dynamics simulation. *Journal of the Chemical Society, Faraday Transactions*, **1996**, 92, 2285		14
1	Genomic and structural features of the Yellow Fever virus from the 2016-2017 Brazilian outbreak		1