Ernesto R Caffarena

List of Publications by Year
in descending order

72 papers	1,365 citations	448610 19 h-index	406436 35 g-index
75 all docs	75 docs citations	75 times ranked	2545 citing authors

#	Article	IF	Citations
1	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, 2022, 40, 10359-10372.	2.0	3
2	In silico investigation of riboswitches in fungi: structural and dynamical insights into TPP riboswitches in Aspergillus oryzae. RNA Biology, 2022, 19, 90-103.	1.5	2
3	Bacterial 2â€²-Deoxyguanosine Riboswitch Classes as Potential Targets for Antibiotics: A Structure and Dynamics Study. International Journal of Molecular Sciences, 2022, 23, 1925.	1.8	3
4	Development of New Potential Inhibitors of Î²1 Integrins through In Silico Methodsâ€”Screening and Computational Validation. Life, 2022, 12, 932.	1.1	4
5	Differences in Charge Distribution in Leishmania tarentolae Leishmanolysin Result in a Reduced Enzymatic Activity. International Journal of Molecular Sciences, 2022, 23, 7660.	1.8	1
6	How does Î±1Histidine102 affect the binding of modulators to Î±1Î²2Î³2 GABAA receptors? molecular insights from in silico experiments. Physical Chemistry Chemical Physics, 2021, 23, 3993-4006.	1.3	2
7	Studying effects of different protonation states of His11 and His102 in ribose-5-phosphate isomerase of Trypanosoma cruzi: an example of cooperative behavior. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2047-2056.	2.0	4
8	Guidelines To Predict Binding Poses of Antibodyâ€“Integrin Complexes. ACS Omega, 2020, 5, 16379-16385.	1.6	1
9	Shared Binding Mode of Perrottetinene and Tetrahydrocannabinol Diastereomers inside the CB1 Receptor May Incentivize Novel Medicinal Drug Design: Findings from an in Silico Assay. ACS Chemical Neuroscience, 2020, 11, 4289-4300.	1.7	3
10	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.	1.6	4
11	Structural insights into NS5B protein of novel equine hepaciviruses and pegiviruses complexed with polymerase inhibitors. Virus Research, 2020, 278, 197867.	1.1	8
12	The rare lncRNA GOLLD is widespread and structurally conserved among Mycobacterium tRNA arrays. RNA Biology, 2020, 17, 1001-1008.	1.5	1
13	Mycobacterium tuberculosis and M. bovis BCG Moreau Fumarate Reductase Operons Produce Different Polypeptides That May Be Related to Non-canonical Functions. Frontiers in Microbiology, 2020, 11, 624121.	1.5	3
14	Effects of the Q80K Polymorphism on the Physicochemical Properties of Hepatitis C Virus Subtype 1a NS3 Protease. Viruses, 2019, 11, 691.	1.5	1
15	Identification of Novel and Recurrent RMRP Variants in a Series of Brazilian Patients with Cartilage-Hair Hypoplasia: McKusick Syndrome. Molecular Syndromology, 2019, 10, 255-263.	0.3	3
16	Integrating Molecular Docking and Molecular Dynamics Simulations. Methods in Molecular Biology, 2019, 2053, 13-34.	0.4	87
17	Benzimidazole inhibitors of the major cysteine protease of Trypanosoma brucei. Future Medicinal Chemistry, 2019, 11, 1537-1551.	1.1	7
18	In silico analysis of the V66M variant of human BDNF in psychiatric disorders: An approach to precision medicine. PLoS ONE, 2019, 14, e0215508.	1.1	24

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19	Unraveling RNA dynamical behavior of TPP riboswitches: a comparison between Escherichia coli and Arabidopsis thaliana. Scientific Reports, 2019, 9, 4197.	1.6	17
20	The role of hydrophobicity in the cold denaturation of proteins under high pressure: A study on apomyoglobin. Journal of Chemical Physics, 2019, 150, 075102.	1.2	6
21	Understanding Structureâ€“Activity Relationships for Trypanosomal Cysteine Protease Inhibitors by Simulations and Free Energy Calculations. Journal of Chemical Information and Modeling, 2019, 59, 137-148.	2.5	17
22	Thiophenacetamide as a potential modulator to NF-ÎºB: structure and dynamics study using in silico and molecular biology assays. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4395-4406.	2.0	3
23	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, 2019, 18, 1457-1468.	0.9	2
24	Pressure effect on micellization of non-ionic surfactant Triton X-100. Journal of Chemical Physics, 2018, 148, 074901.	1.2	6
25	Using RNA Sequence and Structure for the Prediction of Riboswitch Aptamer: A Comprehensive Review of Available Software and Tools. Frontiers in Genetics, 2018, 8, 231.	1.1	31
26	Genomic and structural features of the yellow fever virus from the 2016â€“2017 Brazilian outbreak. Journal of General Virology, 2018, 99, 536-548.	1.3	50
27	Essential dynamics of the cold denaturation: pressure and temperature effects in yeast frataxin. Proteins: Structure, Function and Bioinformatics, 2017, 85, 125-136.	1.5	11
28	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.	2.6	60
29	Structural insights into leishmanolysins encoded on chromosome 10 of Leishmania (Viannia) braziliensis. Memorias Do Instituto Oswaldo Cruz, 2017, 112, 617-625.	0.8	7
30	CaracterizaÃ§Ã£o do envelhecimento populacional no municÃpio do Rio de Janeiro: contribuiÃ§Ãµes para polÃticas pÃºblicas sustentÃ¡veis. Cadernos Saude Coletiva, 2016, 24, 63-69.	0.2	9
31	Exploring the unbinding ofLeishmania(L.)amazonensisCPB derived-epitopes from H2 MHC class I proteins. Proteins: Structure, Function and Bioinformatics, 2016, 84, 473-487.	1.5	14
32	The influence of the pentoseâ€™s pathway of the Clostridium Acetobutylicum on the production of butanol: Insights from mathematical modeling. AIP Conference Proceedings, 2016, , .	0.3	0
33	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.	1.3	2
34	Arising of Simeprevir Drug-Resistance Q80K in Hepatitis C Virus Subtype 1A Clade 2 Isolates. Journal of Hepatology, 2016, 64, S411.	1.8	0
35	Boosting Docking-Based Virtual Screening with Deep Learning. Journal of Chemical Information and Modeling, 2016, 56, 2495-2506.	2.5	265
36	Computational drug design strategies applied to the modelling of human immunodeficiency virus-1 reverse transcriptase inhibitors. Memorias Do Instituto Oswaldo Cruz, 2015, 110, 847-864.	0.8	23

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37	Epoxy-Î±-Lapachone 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, 1910-1918.	1.4	31
38	Gedunin Binds to Myeloid Differentiation Protein 2 and Impairs Lipopolysaccharide-Induced Toll-Like Receptor 4 Signaling in Macrophages. Molecular Pharmacology, 2015, 88, 949-961.	1.0	16
39	<i>In Silico</i> Identification of Novel APRIL Peptide Antagonists and Binding Insights by Molecular Modeling and Immunosorbent Assays. Protein and Peptide Letters, 2015, 22, 432-442.	0.4	1
40	Structural and Molecular Modeling Features of P2X Receptors. International Journal of Molecular Sciences, 2014, 15, 4531-4549.	1.8	24
41	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, 315-323.	0.8	16
42	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.	1.1	15
43	Identifying Drug Repositioning Targets using Text Mining. , 2014, , .		0
44	Mining for Adverse Drug Events on Twitter. , 2014, , .		1
45	Naturally Occurring Genetic Variants of Human Caspase-1 Differ Considerably in Structure and the Ability to Activate Interleukin-1Î². Human Mutation, 2013, 34, 122-131.	1.1	30
46	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, 120-129.	1.9	51
47	PLAUSIBLE BINDING MODE OF THE ACTIVE Î±4Î²1 ANTAGONIST, MK-0617, DETERMINED BY DOCKING AND FREE ENERGY CALCULATIONS. Journal of Theoretical and Computational Chemistry, 2013, 12, 1250108.	1.8	8
48	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, 4333-4341.	0.8	6
49	Computational modeling of the bHLH domain of the transcription factor TWIST1 and R118C, S144R and K145E mutants. BMC Bioinformatics, 2012, 13, 184.	1.2	20
50	Structure-based functional inference of hypothetical proteins from Mycoplasma hyopneumoniae. Journal of Molecular Modeling, 2012, 18, 1917-1925.	0.8	15
51	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.	0.9	26
52	New parameterization approaches of the LIE method to improve free energy calculations of PlmIIâ€Inhibitors complexes. Journal of Computational Chemistry, 2010, 31, 2723-2734.	1.5	15
53	Analysis of Î±4 Î²1integrin 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.	0.6	7
54	Estudo de RepresentaÃ§Ãµes em Redes Neurais para AnÃ¡lise da Afinidade de LigaÃ§Ã£o de Compostos Anti-HIV. Learning and Nonlinear Models, 2010, 8, 52-62.	0.2	0

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55	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.	0.6	8
56	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.	1.2	9
57	Synthesis, antimalarial evaluation and molecular modeling studies of hydroxyethylpiperazines, potential aspartyl protease inhibitors, Part 2. European Journal of Medicinal Chemistry, 2009, 44, 3816-3820.	2.6	24
58	Predictions Suggesting a Participation of Î²-Sheet Configuration in the M2 Domain of the P2X7 Receptor: A Novel Conformation?. Biophysical Journal, 2009, 96, 951-963.	0.2	5
59	Studies of molecular docking between fibroblast growth factor and heparin using generalized simulated annealing. International Journal of Quantum Chemistry, 2008, 108, 2608-2614.	1.0	11
60	Molecular docking study and development of an empirical binding free energy model for phosphodiesterase 4 inhibitors. Bioorganic and Medicinal Chemistry, 2006, 14, 6001-6011.	1.4	15
61	Conformational and dynamical properties of the niruriside in aqueous solution: a molecular dynamics approach. Computational and Theoretical Chemistry, 2005, 714, 189-197.	1.5	3
62	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, 1527-1533.	0.9	140
63	On the hydrogen bond structure of water at different densities. Physica A: Statistical Mechanics and Its Applications, 2004, 342, 34-39.	1.2	21
64	Stochastic molecular dynamics of peanut lectin PNA complex with T-antigen disaccharide. Journal of Molecular Graphics and Modelling, 2002, 21, 227-240.	1.3	8
65	Hydration of T-antigen GalÎ²(1-3)GalNAc and the isomer GalÎ²(1-3)GlcNAc by molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2000, 18, 119-125.	1.3	4
66	Hydration of glucose in the rubbery and glassy states studied by molecular dynamics simulation. Carbohydrate Research, 1999, 315, 63-69.	1.1	36
67	Computer simulation of the cyclodextrinâ€“phenylalanine complex. Carbohydrate Research, 1998, 310, 253-259.	1.1	17
68	Title is missing!. Journal of Solution Chemistry, 1998, 27, 935-948.	0.6	35
69	Hydration properties of xylitol: computer simulation. International Journal of Biological Macromolecules, 1998, 23, 149-155.	3.6	11
70	Glass transition in aqueous solutions of glucose. Molecular dynamics simulation. Carbohydrate Research, 1997, 300, 51-57.	1.1	36
71	Crystal, melted and glassy states of glucose. A molecular dynamics simulation. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2285.	1.7	15
72	REDES NEURAIS PARA ANÃŁISE DA AFINIDADE DE LIGAÃ‡ÃƒO DE COMPOSTOS ANTI-HIV. , 0, , .		0