Rafaela S Ferreira

List of Publications by Year
in descending order

78 papers	2,874 citations	186254 28 h-index	189881 50 g-index
84 all docs	84 docs citations	84 times ranked	3942 citing authors

#	Article	IF	Citations
1	A higher flexibility at the SARS-CoV-2 main protease active site compared to SARS-CoV and its potentialities for new inhibitor virtual screening targeting multi-conformers. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9214-9234.	3.5	7
2	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.	3.5	3
3	Impact of different protonation states on virtual screening performance against cruzain. Chemical Biology and Drug Design, 2022, 99, 703-716.	3.2	1
4	Characterization of an Allosteric Pocket in Zika Virus NS2B-NS3 Protease. Journal of Chemical Information and Modeling, 2022, 62, 945-957.	5.4	4
5	Computational approaches towards the discovery and optimisation of cruzain inhibitors. Memorias Do Instituto Oswaldo Cruz, 2022, 117, e210385.	1.6	8
6	S. mansoni SmKI-1 Kunitz-domain: Leucine point mutation at P1 site generates enhanced neutrophil elastase inhibitory activity. PLoS Neglected Tropical Diseases, 2021, 15, e0009007.	3.0	4
7	Reenacting the Birth of a Function: Functional Divergence of HIUases and Transthyretins as Inferred by Evolutionary and Biophysical Studies. Journal of Molecular Evolution, 2021, 89, 370-383.	1.8	1
8	PyAutoFEP: An Automated Free Energy Perturbation Workflow for GROMACS Integrating Enhanced Sampling Methods. Journal of Chemical Theory and Computation, 2021, 17, 4262-4273.	5.3	23
9	4-Chlorophenylthioacetone-derived thiosemicarbazones as potent antitrypanosomal drug candidates: Investigations on the mode of action. Bioorganic Chemistry, 2021, 113, 105018.	4.1	8
10	Dengue virus 3 genotype I shows natural changes in heparan sulphate binding sites, cell interactions, and neurovirulence in a mouse model. Journal of General Virology, 2021, 102, .	2.9	3
11	Structure-Based Optimization of Quinazolines as Cruzain and TbrCATL Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 13054-13071.	6.4	19
12	The gene repertoire of the main cysteine protease of Trypanosoma cruzi, cruzipain, reveals four sub-types with distinct active sites. Scientific Reports, 2021, 11, 18231.	3.3	16
13	Multiparameter Optimization of Trypanocidal Cruzain Inhibitors With In Vivo Activity and Favorable Pharmacokinetics. Frontiers in Pharmacology, 2021, 12, 774069.	3.5	6
14	Discovery of Potent, Reversible, and Competitive Cruzain Inhibitors with Trypanocidal Activity: A Structure-Based Drug Design Approach. Journal of Chemical Information and Modeling, 2020, 60, 1028-1041.	5.4	32
15	Profiling selectivity of chagasin mutants towards cysteine proteases cruzain or cathepsin L through molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-13.	3.5	1
16	Antigenic and Substrate Preference Differences between Scorpion and Spider Dermonecrotic Toxins, a Comparative Investigation. Toxins, 2020, 12, 631.	3.4	7
17	Synthesis of quinoline derivatives as potential cysteine protease inhibitors. Future Medicinal Chemistry, 2020, 12, 571-581.	2.3	9
18	Cruzain structures: apocruzain and cruzain bound to S-methyl thiomethanesulfonate and implications for drug design. Acta Crystallographica Section F, Structural Biology Communications, 2019, 75, 419-427.	0.8	11

#	Article	IF	Citations
19	2-(phenylthio)ethylidene derivatives as anti-Trypanosoma cruzi compounds: Structural design, synthesis and antiparasitic activity. European Journal of Medicinal Chemistry, 2019, 180, 191-203.	5.5	14
20	Benzimidazole inhibitors of the major cysteine protease of Trypanosoma brucei. Future Medicinal Chemistry, 2019, 11, 1537-1551.	2.3	7
21	Discovery and characterization of trypanocidal cysteine protease inhibitors from the â€˜malaria boxâ€™. European Journal of Medicinal Chemistry, 2019, 179, 765-778.	5.5	19
22	JVA, an isoniazid analogue, is a bioactive compound against a clinical isolate of the Mycobacterium avium complex. Tuberculosis, 2019, 115, 108-112.	1.9	2
23	Insights into Substrate and Inhibitor Selectivity among Human GLUT Transporters through Comparative Modeling and Molecular Docking. ACS Omega, 2019, 4, 4748-4760.	3.5	7
24	Design, Synthesis and In Vitro Trypanocidal and Leishmanicidal Activities of 2â€(2â€Arylidene)hydrazonoâ€4â€oxothiazolidineâ€5â€acetic Acid Derivatives. ChemistrySelect, 2019, 4, 13163-13172.	1.5	7
25	Structure-Based and Molecular Modeling Studies for the Discovery of Cyclic Imides as Reversible Cruzain Inhibitors With Potent Anti-Trypanosoma cruzi Activity. Frontiers in Chemistry, 2019, 7, 798.	3.6	24
26	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.	5.4	17
27	nAPOLI: a graph-based strategy to detect and visualize conserved protein-ligand interactions in large-scale. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2019, 17, 1-1.	3.0	25
28	Structure-based Approaches Targeting Parasite Cysteine Proteases. Current Medicinal Chemistry, 2019, 26, 4435-4453.	2.4	10
29	Zirconium catalyzed synthesis of 2-arylidene Indan-1,3-diones and evaluation of their inhibitory activity against NS2B-NS3 WNV protease. European Journal of Medicinal Chemistry, 2018, 149, 98-109.	5.5	22
30	Synthesis and leishmanicidal activity of eugenol derivatives bearing 1,2,3-triazole functionalities. European Journal of Medicinal Chemistry, 2018, 146, 274-286.	5.5	49
31	Investigation of the binding mode of a novel cruzain inhibitor by docking, molecular dynamics, ab initio and MM/PBSA calculations. Journal of Computer-Aided Molecular Design, 2018, 32, 591-605.	2.9	18
32	Synthesis and structure-activity relationship studies of cruzain and rhodesain inhibitors. European Journal of Medicinal Chemistry, 2018, 157, 1426-1459.	5.5	32
33	Antimetastatic effect of the pharmacological inhibition of serine/arginine-rich protein kinases (SRPK) in murine melanoma. Toxicology and Applied Pharmacology, 2018, 356, 214-223.	2.8	17
34	Ortho-nitrobenzyl derivatives as potential anti-schistosomal agents. Brazilian Journal of Pharmaceutical Sciences, 2018, 54, .	1.2	6
35	Schistosoma mansoni SmKI-1 serine protease inhibitor binds to elastase and impairs neutrophil function and inflammation. PLoS Pathogens, 2018, 14, e1006870.	4.7	58
36	Structure-Based Virtual Screening and Biochemical Evaluation for the Identification of Novel Trypanosoma brucei Aldolase Inhibitors. Current Topics in Medicinal Chemistry, 2018, 18, 397-405.	2.1	5

#	Article	IF	Citations
37	Application of bioisosterism in design of the semicarbazone derivatives as cruzain inhibitors: a theoretical and experimental study. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1244-1259.	3.5	14
38	Synthesis and biological evaluation of potential inhibitors of the cysteine proteases cruzain and rhodesain designed by molecular simplification. Bioorganic and Medicinal Chemistry, 2017, 25, 1889-1900.	3.0	39
39	Desing and synthesis of potent anti-Trypanosoma cruzi agents new thiazoles derivatives which induce apoptotic parasite death. European Journal of Medicinal Chemistry, 2017, 130, 39-50.	5.5	40
40	Molecular modeling and structureâ€“activity relationships for a series of benzimidazole derivatives as cruzain inhibitors. Future Medicinal Chemistry, 2017, 9, 641-657.	2.3	18
41	Structural design, synthesis and pharmacological evaluation of thiazoles against Trypanosoma cruzi. European Journal of Medicinal Chemistry, 2017, 141, 346-361.	5.5	43
42	Corynebacterium pseudotuberculosis may be under anagenesis and biovar Equi forms biovar Ovis: a phylogenic inference from sequence and structural analysis. BMC Microbiology, 2016, 16, 100.	3.3	11
43	Open Source Drug Discovery with the Malaria Box Compound Collection for Neglected Diseases and Beyond. PLoS Pathogens, 2016, 12, e1005763.	4.7	244
44	New 1,3-thiazole derivatives and their biological and ultrastructural effects on Trypanosoma cruzi. European Journal of Medicinal Chemistry, 2016, 121, 387-398.	5.5	46
45	Design, synthesis, molecular docking and biological evaluation of thiophen-2-iminothiazolidine derivatives for use against Trypanosoma cruzi. Bioorganic and Medicinal Chemistry, 2016, 24, 4228-4240.	3.0	38
46	In silico identification of essential proteins in Corynebacterium pseudotuberculosis based on protein-protein interaction networks. BMC Systems Biology, 2016, 10, 103.	3.0	24
47	Unraveling the distinctive features of hemorrhagic and non-hemorrhagic snake venom metalloproteinases using molecular simulations. Journal of Computer-Aided Molecular Design, 2016, 30, 69-83.	2.9	4
48	An integrated structural proteomics approach along the druggable genome of Corynebacterium pseudotuberculosis species for putative druggable targets. BMC Genomics, 2015, 16, S9.	2.8	25
49	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.	1.6	23
50	Synthesis of a Sugar-Based Thiosemicarbazone Series and Structure-Activity Relationship versus the Parasite Cysteine Proteases Rhodesain, Cruzain, and Schistosoma mansoni Cathepsin B1. Antimicrobial Agents and Chemotherapy, 2015, 59, 2666-2677.	3.2	57
51	Synthesis and structureâ€“activity relationship study of a new series of antiparasitic aryloxyl thiosemicarbazones inhibiting Trypanosoma cruzi cruzain. European Journal of Medicinal Chemistry, 2015, 101, 818-835.	5.5	54
52	Structural design, synthesis and pharmacological evaluation of 4-thiazolidinones against Trypanosoma cruzi. Bioorganic and Medicinal Chemistry, 2015, 23, 7478-7486.	3.0	35
53	In Silico Protein-Protein Interactions: Avoiding Data and Method Biases Over Sensitivity and Specificity. Current Protein and Peptide Science, 2015, 16, 689-700.	1.4	8
54	An improved interolog mapping-based computational prediction of proteinâ€“protein interactions with increased network coverage. Integrative Biology (United Kingdom), 2014, 6, 1080-1087.	1.3	32

#	Article	IF	Citations
55	Conformational restriction of aryl thiosemicarbazones produces potent and selective anti-Trypanosoma cruzi compounds which induce apoptotic parasite death. European Journal of Medicinal Chemistry, 2014, 75, 467-478.	5.5	46
56	Synthesis and evaluation of the antiparasitic activity of bis-(arylmethylidene) cycloalkanones. European Journal of Medicinal Chemistry, 2014, 71, 282-289.	5.5	43
57	Structural Design, Synthesis and Structureâ€“Activity Relationships of Thiazolidinones with Enhanced Antiâ€Trypanosoma cruzi Activity. ChemMedChem, 2014, 9, 177-188.	3.2	39
58	2-Pyridyl thiazoles as novel anti-Trypanosoma cruzi agents: Structural design, synthesis and pharmacological evaluation. European Journal of Medicinal Chemistry, 2014, 86, 48-59.	5.5	86
59	Synthesis, Biological Evaluation, and Structureâ€“Activity Relationships of Potent Noncovalent and Nonpeptidic Cruzain Inhibitors as Anti-Trypanosoma cruzi Agents. Journal of Medicinal Chemistry, 2014, 57, 2380-2392.	6.4	62
60	Proteome scale comparative modeling for conserved drug and vaccine targets identification in Corynebacterium pseudotuberculosis. BMC Genomics, 2014, 15, S3.	2.8	30
61	Structure-Based Drug Design to Overcome Drug Resistance: Challenges and Opportunities. Current Pharmaceutical Design, 2014, 20, 687-693.	1.9	5
62	Structural Investigation of Anti-Trypanosoma cruzi 2-Iminothiazolidin-4-ones Allows the Identification of Agents with Efficacy in Infected Mice. Journal of Medicinal Chemistry, 2012, 55, 10918-10936.	6.4	55
63	Optimization of anti-Trypanosoma cruzi oxadiazoles leads to identification of compounds with efficacy in infected mice. Bioorganic and Medicinal Chemistry, 2012, 20, 6423-6433.	3.0	37
64	In silicoscreening strategies for novel inhibitors of parasitic diseases. Expert Opinion on Drug Discovery, 2011, 6, 481-489.	5.0	10
65	IntegraÃ§Ã£o das tÃ©cnicas de triagem virtual e triagem biolÃ³gica automatizada em alta escala: oportunidades e desafios em P&D de fÃ¡rmacos. Quimica Nova, 2011, 34, 1770-1778.	0.3	19
66	Studies toward the structural optimization of novel thiazolylhydrazone-based potent antitrypanosomal agents. Bioorganic and Medicinal Chemistry, 2010, 18, 7826-7835.	3.0	46
67	Identification and Optimization of Inhibitors of Trypanosomal Cysteine Proteases: Cruzain, Rhodesain, and TbCatB. Journal of Medicinal Chemistry, 2010, 53, 52-60.	6.4	103
68	Quantitative Analyses of Aggregation, Autofluorescence, and Reactivity Artifacts in a Screen for Inhibitors of a Thiol Protease. Journal of Medicinal Chemistry, 2010, 53, 37-51.	6.4	213
69	Complementarity Between a Docking and a High-Throughput Screen in Discovering New Cruzain Inhibitors. Journal of Medicinal Chemistry, 2010, 53, 4891-4905.	6.4	199
70	Two approaches to discovering and developing new drugs for Chagas disease. Memorias Do Instituto Oswaldo Cruz, 2009, 104, 263-269.	1.6	137
71	Docking and chemoinformatic screens for new ligands and targets. Current Opinion in Biotechnology, 2009, 20, 429-436.	6.6	168
72	Novel non-peptidic vinylsulfones targeting the S2 and S3 subsites of parasite cysteine proteases. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 6218-6221.	2.2	56

#	Article	IF	Citations
73	Divergent Modes of Enzyme Inhibition in a Homologous Structureâ˜Activity Series. Journal of Medicinal Chemistry, 2009, 52, 5005-5008.	6.4	84
74	Docking for fragment inhibitors of AmpC Î²-lactamase. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 7455-7460.	7.1	101
75	SÃntese, avaliaÃ§Ã£o biolÃ³gica e modelagem molecular de arilfuranos como inibidores da enzima tripanotiona redutase. Quimica Nova, 2008, 31, 261-267.	0.3	16
76	A Mitogenic Protein Fraction in Latex fromCarica candamarcensis. Planta Medica, 2003, 69, 926-932.	1.3	20
77	In vitro study on thiabendazole action on viability of Ascaris lumbricoides (Lineu, 1758) eggs. Revista Da Sociedade Brasileira De Medicina Tropical, 2001, 34, 319-322.	0.9	9
78	Carbamoyl Imidazoles As Potent, Reversible and Competitive Cruzain Inhibitors with in vitro and in vivo Trypanocidal Activity: A Structure-Based Drug Design Approach. SSRN Electronic Journal, 0, , .	0.4	0