AdriÃ¡n Gustavo Turjanski

List of Publications by Year
in descending order

86 papers	2,896 citations	172457 29 h-index	197818 49 g-index
91 all docs	91 docs citations	91 times ranked	4670 citing authors

#	Article	IF	Citations
1	Specificity and Reactivity of Mycobacterium tuberculosis Serine/Threonine Kinases PknG and PknB. Journal of Chemical Information and Modeling, 2022, 62, 1723-1733.	5.4	3
2	Development of an Improved Guanidineâ€Based Rac1 Inhibitor with inâ€…vivo Activity against Nonâ€Small Cell Lung Cancer. ChemMedChem, 2021, 16, 1011-1021.	3.2	12
3	Oculocutaneous albinism type 1B associated with a functionally significant tyrosinase gene polymorphism detected with Whole Exome Sequencing. Ophthalmic Genetics, 2021, 42, 291-295.	1.2	3
4	Five-year microevolution of a multidrug-resistant Mycobacterium tuberculosis strain within a patient with inadequate compliance to treatment. BMC Infectious Diseases, 2021, 21, 394.	2.9	3
5	Six novel variants in the PKLR gene associated with pyruvate kinase deficiency in Argentinian patients. Clinical Biochemistry, 2021, 91, 26-30.	1.9	7
6	Conformational and Reaction Dynamic Coupling in Histidine Kinases: Insights from Hybrid QM/MM Simulations. Journal of Chemical Information and Modeling, 2020, 60, 833-842.	5.4	8
7	MRSA dynamic circulation between the community and the hospital setting: New insights from a cohort study. Journal of Infection, 2020, 80, 24-37.	3.3	17
8	Kinase Activation by Small Conformational Changes. Journal of Chemical Information and Modeling, 2020, 60, 821-832.	5.4	15
9	New one-pot synthesis of anti-tuberculosis compounds inspired on isoniazid. European Journal of Medicinal Chemistry, 2020, 208, 112699.	5.5	21
10	A novel mutation in PSEN1 (p.Arg41Ser) in an Argentinian woman with early onset Parkinsonism. Parkinsonism and Related Disorders, 2020, 77, 21-25.	2.2	13
11	Aromatic clusters in proteinâ€“protein and proteinâ€“drug complexes. Journal of Cheminformatics, 2020, 12, 30.	6.1	38
12	Cosolvent-Based Protein Pharmacophore for Ligand Enrichment in Virtual Screening. Journal of Chemical Information and Modeling, 2019, 59, 3572-3583.	5.4	21
13	Reverse Engineering of an Aspirin-Responsive Transcriptional Regulator in Escherichia coli. ACS Synthetic Biology, 2019, 8, 1890-1900.	3.8	13
14	Toward unrestricted use of public genomic data. Science, 2019, 363, 350-352.	12.6	45
15	Consent insufficient for data releaseâ€”Response. Science, 2019, 364, 446-446.	12.6	5
16	Target-Pathogen: a structural bioinformatic approach to prioritize drug targets in pathogens. Nucleic Acids Research, 2018, 46, D413-D418.	14.5	53
17	Characterization and comparative analysis of the genome of Puccinia sorghi Schwein, the causal agent of maize common rust. Fungal Genetics and Biology, 2018, 112, 31-39.	2.1	31
18	Structural and mechanistic comparison of the Cyclopropane Mycolic Acid Synthases (CMAS) protein family of Mycobacterium tuberculosis. Biochemical and Biophysical Research Communications, 2018, 498, 288-295.	2.1	8

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19	Multiscale approach to the activation and phosphotransfer mechanism of CpxA histidine kinase reveals a tight coupling between conformational and chemical steps. Biochemical and Biophysical Research Communications, 2018, 498, 305-312.	2.1	11
20	VarQ: A Tool for the Structural and Functional Analysis of Human Protein Variants. Frontiers in Genetics, 2018, 9, 620.	2.3	10
21	Solvents to Fragments to Drugs: MD Applications in Drug Design. Molecules, 2018, 23, 3269.	3.8	25
22	Genetics and genomic medicine in Argentina. Molecular Genetics & Genomic Medicine, 2018, 6, 481-491.	1.2	17
23	The Druggable Pocketome of Corynebacterium diphtheriae: A New Approach for in silico Putative Druggable Targets. Frontiers in Genetics, 2018, 9, 44.	2.3	8
24	Fluoromycobacteriophages Can Detect Viable Mycobacterium tuberculosis and Determine Phenotypic Rifampicin Resistance in 3â€“5 Days From Sputum Collection. Frontiers in Microbiology, 2018, 9, 1471.	3.5	18
25	An integrative, multi-omics approach towards the prioritization of Klebsiella pneumoniae drug targets. Scientific Reports, 2018, 8, 10755.	3.3	50
26	Molecular Dynamics in Mixed Solvents Reveals Proteinâ€“Ligand Interactions, Improves Docking, and Allows Accurate Binding Free Energy Predictions. Journal of Chemical Information and Modeling, 2017, 57, 846-863.	5.4	68
27	First Whole-Genome Shotgun Sequence of a Promising Cellulase Secretor, Trichoderma koningiopsis Strain POS7. Genome Announcements, 2017, 5, .	0.8	7
28	LigQ: A Webserver to Select and Prepare Ligands for Virtual Screening. Journal of Chemical Information and Modeling, 2017, 57, 1741-1746.	5.4	5
29	An integrative in-silico approach for therapeutic target identification in the human pathogen Corynebacterium diphtheriae. PLoS ONE, 2017, 12, e0186401.	2.5	35
30	Structural and functional characterization of a coldâ€adapted standâ€alone <scp>TPM</scp> domain reveals a relationship between dynamics and phosphatase activity. FEBS Journal, 2016, 283, 4370-4385.	4.7	4
31	Structured and Unstructured Binding of an Intrinsically Disordered Protein as Revealed by Atomistic Simulations. Journal of the American Chemical Society, 2016, 138, 8742-8751.	13.7	32
32	Two novel DNA variants associated with glucose-6-phosphate dehydrogenase deficiency found in Argentine pediatric patients. Clinical Biochemistry, 2016, 49, 808-810.	1.9	3
33	Phosphorylation or Mutation of the ERK2 Activation Loop Alters Oligonucleotide Binding. Biochemistry, 2016, 55, 1909-1917.	2.5	12
34	A whole genome bioinformatic approach to determine potential latent phase specific targets in Mycobacterium tuberculosis. Tuberculosis, 2016, 97, 181-192.	1.9	21
35	Phosphorylation Regulates the Bound Structure of an Intrinsically Disordered Protein: The p53-TAZ2 Case. PLoS ONE, 2016, 11, e0144284.	2.5	16
36	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

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37	Genome comparison of two Exiguobacterium strains from high altitude andean lakes with different arsenic resistance: identification and 3D modeling of the Acr3 efflux pump. Frontiers in Environmental Science, 2015, 3, .	3.3	54
38	Whole Genome Sequencing Reveals a De Novo SHANK3 Mutation in Familial Autism Spectrum Disorder. PLoS ONE, 2015, 10, e0116358.	2.5	55
39	A Novel Missense Mutation in theHSD3B2Gene, Underlying Nonsalt-Wasting Congenital Adrenal Hyperplasia. New Insight Into the Structure-Function Relationships of 3Î²-Hydroxysteroid Dehidrogenase Type II. Journal of Clinical Endocrinology and Metabolism, 2015, 100, E191-E196.	3.6	10
40	MAPKâ€™s networks and their capacity for multistationarity due to toric steady states. Mathematical Biosciences, 2015, 262, 125-137.	1.9	14
41	WATCLUST: a tool for improving the design of drugs based on protein-water interactions. Bioinformatics, 2015, 31, 3697-3699.	4.1	47
42	A computational study of the interaction of the foot and mouth disease virus VP1 with monoclonal antibodies. Journal of Immunological Methods, 2015, 425, 51-57.	1.4	3
43	Protein Topology Determines Cysteine Oxidation Fate: The Case of Sulfenyl Amide Formation among Protein Families. PLoS Computational Biology, 2015, 11, e1004051.	3.2	39
44	Using crystallographic water properties for the analysis and prediction of lectin-carbohydrate complex structures. Glycobiology, 2015, 25, 181-196.	2.5	19
45	Preclinical Development of Novel Rac1-GEF Signaling Inhibitors using a Rational Design Approach in Highly Aggressive Breast Cancer Cell Lines. Anti-Cancer Agents in Medicinal Chemistry, 2014, 14, 840-851.	1.7	67
46	Draft Genome Sequence of the Polyextremophilic Halorubrum sp. Strain AJ67, Isolated from Hyperarsenic Lakes in the Argentinian Puna. Genome Announcements, 2014, 2, .	0.8	12
47	TuberQ: a Mycobacterium tuberculosis protein druggability database. Database: the Journal of Biological Databases and Curation, 2014, 2014, bau035-bau035.	3.0	35
48	Thiol redox biochemistry: insights from computer simulations. Biophysical Reviews, 2014, 6, 27-46.	3.2	29
49	QM/MM study of the Câ€”C coupling reaction mechanism of CYP121, an essential Cytochrome p450 of Mycobacterium tuberculosis. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1004-1021.	2.6	28
50	Exposing the Secrets of Two Well-Known Lactobacillus casei Phages, J-1 and PL-1, by Genomic and Structural Analysis. Applied and Environmental Microbiology, 2014, 80, 7107-7121.	3.1	22
51	Solution and crystal structure of BA42, a protein from the Antarctic bacteriumBizionia argentinensiscomprised of a stand-alone TPM domain. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3062-3078.	2.6	8
52	Proteome scale comparative modeling for conserved drug and vaccine targets identification in Corynebacterium pseudotuberculosis. BMC Genomics, 2014, 15, S3.	2.8	30
53	Molecular Dynamics Simulations Provide Atomistic Insight into Hydrogen Exchange Mass Spectrometry Experiments. Journal of Chemical Theory and Computation, 2013, 9, 658-669.	5.3	30
54	Extracellular hydrolytic enzyme production by proteolytic bacteria from the Antarctic. Polish Polar Research, 2013, 34, 253-267.	0.9	14

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55	FUNCTIONAL ANALYSIS OF A MOSQUITO SHORTâ€CHAIN DEHYDROGENASE CLUSTER. Archives of Insect Biochemistry and Physiology, 2013, 82, 96-115.	1.5	16
56	Draft Genome Sequence of the Polyextremophilic Exiguobacterium sp. Strain S17, Isolated from Hyperarsenic Lakes in the Argentinian Puna. Genome Announcements, 2013, 1, .	0.8	57
57	In Silico Structural and Functional Characterization of the RSUME Splice Variants. PLoS ONE, 2013, 8, e57795.	2.5	11
58	Protein frustratometer: a tool to localize energetic frustration in protein molecules. Nucleic Acids Research, 2012, 40, W348-W351.	14.5	135
59	1H, 15N and 13C chemical shift assignments of the BA42 protein of the psychrophilic bacteria Bizionia argentinensis sp. nov. Biomolecular NMR Assignments, 2012, 6, 181-183.	0.8	3
60	The Crystal Structure of the MAP Kinase LmaMPK10 from Leishmania Major Reveals Parasite-Specific Features and Regulatory Mechanisms. Structure, 2012, 20, 1649-1660.	3.3	19
61	Culturable heterotrophic bacteria from Potter Cove, Antarctica, and their hydrolytic enzymes production. Polar Research, 2012, 31, 18507.	1.6	22
62	p38Î³ Activation Triggers Dynamical Changes in Allosteric Docking Sites. Biochemistry, 2011, 50, 1384-1395.	2.5	11
63	Genome Sequence of Sphingomonas sp. S17, Isolated from an Alkaline, Hyperarsenic, and Hypersaline Volcano-Associated Lake at High Altitude in the Argentinean Puna. Journal of Bacteriology, 2011, 193, 3686-3687.	2.2	38
64	Juvenile hormone synthesis: â€œesterify then epoxidizeâ€•or â€œepoxidize then esterifyâ€? Insights from the structural characterization of juvenile hormone acid methyltransferase. Insect Biochemistry and Molecular Biology, 2011, 41, 228-235.	2.7	42
65	Aromaticâ€“Aromatic Interactions in Proteins: Beyond the Dimer. Journal of Chemical Information and Modeling, 2011, 51, 1623-1633.	5.4	115
66	Draft Genome Sequence of Bizionia argentinensis, Isolated from Antarctic Surface Water. Journal of Bacteriology, 2011, 193, 6797-6798.	2.2	12
67	Exploration and optimization of substituted triazolothiadiazines and triazolopyridazines as PDE4 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 3686-3692.	2.2	44
68	Molecular and functional characterization of a juvenile hormone acid methyltransferase expressed in the corpora allata of mosquitoes. Insect Biochemistry and Molecular Biology, 2009, 39, 31-37.	2.7	55
69	How Mitogen-Activated Protein Kinases Recognize and Phosphorylate Their Targets: A QM/MM Study. Journal of the American Chemical Society, 2009, 131, 6141-6148.	13.7	43
70	NMR and molecular dynamics studies of the interaction of melatonin with calmodulin. Protein Science, 2008, 13, 2925-2938.	7.6	40
71	Binding-Induced Folding of a Natively Unstructured Transcription Factor. PLoS Computational Biology, 2008, 4, e1000060.	3.2	189
72	MAP kinases and the control of nuclear events. Oncogene, 2007, 26, 3240-3253.	5.9	371

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73	Investigation of the Catalytic Mechanism of Farnesyl Pyrophosphate Synthase by Computer Simulation. Journal of Physical Chemistry B, 2006, 110, 18052-18057.	2.6	23
74	Characterization of the farnesyl pyrophosphate synthase of Trypanosoma cruzi by homology modeling and molecular dynamics. Journal of Molecular Graphics and Modelling, 2006, 25, 345-352.	2.4	17
75	Mechanisms of NO Release by N1-Nitrosomelatonin:â€‰ Nucleophilic Attack versus Reducing Pathways. Journal of Organic Chemistry, 2005, 70, 5790-5798.	3.2	28
76	Transnitrosation of Nitrosothiols:Â Characterization of an Elusive Intermediate. Journal of the American Chemical Society, 2005, 127, 486-487.	13.7	51
77	Ab Initio Study of NMR15N Chemical Shift Differences Induced by Ca2+Binding to EF-Hand Proteinsâ€. Biochemistry, 2004, 43, 6554-6564.	2.5	14
78	Physiological concentrations of melatonin inhibit the nitridergic pathway in the Syrian hamster retina. Journal of Pineal Research, 2002, 33, 31-36.	7.4	47
79	Molecular structure effects on the kinetics of hydroxyl radical addition to azo dyes. Journal of Physical Organic Chemistry, 2002, 15, 287-292.	1.9	19
80	Electronic spectra of indolyl radicals: a time-dependent DFT study. Chemical Physics Letters, 2002, 365, 15-21.	2.6	28
81	Structure, solvation, and bonding in pentacyano(L)ferrate(II) ions (L=aliphatic amine): a density functional study. Journal of Molecular Modeling, 2001, 7, 201-206.	1.8	25
82	Nitrosation of melatonin by nitric oxide: a computational study. Journal of Pineal Research, 2001, 31, 97-101.	7.4	40
83	Stabilization of Aliphatic and Aromatic Diazonium Ions by Coordination:â€‰ An Experimental and Theoretical Study. Organometallics, 2000, 19, 3810-3817.	2.3	22
84	Scavenging of NO by Melatonin. Journal of the American Chemical Society, 2000, 122, 10468-10469.	13.7	80
85	Reactions of Melatonin and Related Indoles with Free Radicals:Â A Computational Study. Journal of Medicinal Chemistry, 1998, 41, 3684-3689.	6.4	73
86	Cosolvent Sites-Based Discovery of Mycobacterium Tuberculosis Protein Kinase G Inhibitors. Journal of Medicinal Chemistry, 0, , .	6.4	3