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	MAP kinases and the control of nuclear events. Oncogene, 2007, 26, 3240-3253.	5.9	371
2	Binding-Induced Folding of a Natively Unstructured Transcription Factor. PLoS Computational Biology, 2008, 4, e1000060.	3.2	189
3	Protein frustratometer: a tool to localize energetic frustration in protein molecules. Nucleic Acids Research, 2012, 40, W348-W351.	14.5	135
4	Aromaticâ€“Aromatic Interactions in Proteins: Beyond the Dimer. Journal of Chemical Information and Modeling, 2011, 51, 1623-1633.	5.4	115
5	Scavenging of NO by Melatonin. Journal of the American Chemical Society, 2000, 122, 10468-10469.	13.7	80
6	Reactions of Melatonin and Related Indoles with Free Radicals:Â A Computational Study. Journal of Medicinal Chemistry, 1998, 41, 3684-3689.	6.4	73
7	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
8	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
9	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
10	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
11	Whole Genome Sequencing Reveals a De Novo SHANK3 Mutation in Familial Autism Spectrum Disorder. PLoS ONE, 2015, 10, e0116358.	2.5	55
12	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
13	Target-Pathogen: a structural bioinformatic approach to prioritize drug targets in pathogens. Nucleic Acids Research, 2018, 46, D413-D418.	14.5	53
14	Transnitrosation of Nitrosothiols:Â Characterization of an Elusive Intermediate. Journal of the American Chemical Society, 2005, 127, 486-487.	13.7	51
15	An integrative, multi-omics approach towards the prioritization of Klebsiella pneumoniae drug targets. Scientific Reports, 2018, 8, 10755.	3.3	50
16	Physiological concentrations of melatonin inhibit the nitridergic pathway in the Syrian hamster retina. Journal of Pineal Research, 2002, 33, 31-36.	7.4	47
17	WATCLUST: a tool for improving the design of drugs based on protein-water interactions. Bioinformatics, 2015, 31, 3697-3699.	4.1	47
18	Toward unrestricted use of public genomic data. Science, 2019, 363, 350-352.	12.6	45

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19	Exploration and optimization of substituted triazolothiadiazines and triazolopyridazines as PDE4 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 3686-3692.	2.2	44
20	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
21	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
22	Nitrosation of melatonin by nitric oxide: a computational study. Journal of Pineal Research, 2001, 31, 97-101.	7.4	40
23	NMR and molecular dynamics studies of the interaction of melatonin with calmodulin. Protein Science, 2008, 13, 2925-2938.	7.6	40
24	Protein Topology Determines Cysteine Oxidation Fate: The Case of Sulfenyl Amide Formation among Protein Families. PLoS Computational Biology, 2015, 11, e1004051.	3.2	39
25	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
26	Aromatic clusters in proteinâ€“protein and proteinâ€“drug complexes. Journal of Cheminformatics, 2020, 12, 30.	6.1	38
27	TuberQ: a Mycobacterium tuberculosis protein druggability database. Database: the Journal of Biological Databases and Curation, 2014, 2014, bau035-bau035.	3.0	35
28	An integrative in-silico approach for therapeutic target identification in the human pathogen Corynebacterium diphtheriae. PLoS ONE, 2017, 12, e0186401.	2.5	35
29	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
30	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
31	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
32	Proteome scale comparative modeling for conserved drug and vaccine targets identification in Corynebacterium pseudotuberculosis. BMC Genomics, 2014, 15, S3.	2.8	30
33	Thiol redox biochemistry: insights from computer simulations. Biophysical Reviews, 2014, 6, 27-46.	3.2	29
34	Electronic spectra of indolyl radicals: a time-dependent DFT study. Chemical Physics Letters, 2002, 365, 15-21.	2.6	28
35	Mechanisms of NO Release by N1-Nitrosomelatonin:â€‰ Nucleophilic Attack versus Reducing Pathways. Journal of Organic Chemistry, 2005, 70, 5790-5798.	3.2	28
36	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

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37	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
38	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
39	Solvents to Fragments to Drugs: MD Applications in Drug Design. Molecules, 2018, 23, 3269.	3.8	25
40	Investigation of the Catalytic Mechanism of Farnesyl Pyrophosphate Synthase by Computer Simulation. Journal of Physical Chemistry B, 2006, 110, 18052-18057.	2.6	23
41	Stabilization of Aliphatic and Aromatic Diazonium Ions by Coordination:â€‰ An Experimental and Theoretical Study. Organometallics, 2000, 19, 3810-3817.	2.3	22
42	Culturable heterotrophic bacteria from Potter Cove, Antarctica, and their hydrolytic enzymes production. Polar Research, 2012, 31, 18507.	1.6	22
43	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
44	A whole genome bioinformatic approach to determine potential latent phase specific targets in Mycobacterium tuberculosis. Tuberculosis, 2016, 97, 181-192.	1.9	21
45	Cosolvent-Based Protein Pharmacophore for Ligand Enrichment in Virtual Screening. Journal of Chemical Information and Modeling, 2019, 59, 3572-3583.	5.4	21
46	New one-pot synthesis of anti-tuberculosis compounds inspired on isoniazid. European Journal of Medicinal Chemistry, 2020, 208, 112699.	5.5	21
47	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
48	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
49	Using crystallographic water properties for the analysis and prediction of lectin-carbohydrate complex structures. Glycobiology, 2015, 25, 181-196.	2.5	19
50	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
51	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
52	Genetics and genomic medicine in Argentina. Molecular Genetics & Genomic Medicine, 2018, 6, 481-491.	1.2	17
53	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
54	FUNCTIONAL ANALYSIS OF A MOSQUITO SHORTâ€CHAIN DEHYDROGENASE CLUSTER. Archives of Insect Biochemistry and Physiology, 2013, 82, 96-115.	1.5	16

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55	Phosphorylation Regulates the Bound Structure of an Intrinsically Disordered Protein: The p53-TAZ2 Case. PLoS ONE, 2016, 11, e0144284.	2.5	16
56	Kinase Activation by Small Conformational Changes. Journal of Chemical Information and Modeling, 2020, 60, 821-832.	5.4	15
57	Ab Initio Study of NMR15N Chemical Shift Differences Induced by Ca2+Binding to EF-Hand Proteinsâ€. Biochemistry, 2004, 43, 6554-6564.	2.5	14
58	Extracellular hydrolytic enzyme production by proteolytic bacteria from the Antarctic. Polish Polar Research, 2013, 34, 253-267.	0.9	14
59	MAPKâ€™s networks and their capacity for multistationarity due to toric steady states. Mathematical Biosciences, 2015, 262, 125-137.	1.9	14
60	Reverse Engineering of an Aspirin-Responsive Transcriptional Regulator in Escherichia coli. ACS Synthetic Biology, 2019, 8, 1890-1900.	3.8	13
61	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
62	Draft Genome Sequence of Bizionia argentinensis, Isolated from Antarctic Surface Water. Journal of Bacteriology, 2011, 193, 6797-6798.	2.2	12
63	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
64	Phosphorylation or Mutation of the ERK2 Activation Loop Alters Oligonucleotide Binding. Biochemistry, 2016, 55, 1909-1917.	2.5	12
65	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
66	p38Î³ Activation Triggers Dynamical Changes in Allosteric Docking Sites. Biochemistry, 2011, 50, 1384-1395.	2.5	11
67	In Silico Structural and Functional Characterization of the RSUME Splice Variants. PLoS ONE, 2013, 8, e57795.	2.5	11
68	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
69	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
70	VarQ: A Tool for the Structural and Functional Analysis of Human Protein Variants. Frontiers in Genetics, 2018, 9, 620.	2.3	10
71	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
72	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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73	The Druggable Pocketome of Corynebacterium diphtheriae: A New Approach for in silico Putative Druggable Targets. Frontiers in Genetics, 2018, 9, 44.	2.3	8
74	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
75	First Whole-Genome Shotgun Sequence of a Promising Cellulase Secretor, Trichoderma koningiopsis Strain POS7. Genome Announcements, 2017, 5, .	0.8	7
76	Six novel variants in the PKLR gene associated with pyruvate kinase deficiency in Argentinian patients. Clinical Biochemistry, 2021, 91, 26-30.	1.9	7
77	LigQ: A Webserver to Select and Prepare Ligands for Virtual Screening. Journal of Chemical Information and Modeling, 2017, 57, 1741-1746.	5.4	5
78	Consent insufficient for data releaseâ€"Response. Science, 2019, 364, 446-446.	12.6	5
79	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
80	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
81	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
82	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
83	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
84	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
85	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
86	Cosolvent Sites-Based Discovery of Mycobacterium Tuberculosis Protein Kinase G Inhibitors. Journal of Medicinal Chemistry, 0, , .	6.4	3