Alejandro Giorgetti

List of Publications by Year
in descending order

100	2,105	257450	289244
papers	citations	24 h-index	40 g-index

104	104	104	3276
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The implications of alternative splicing in the ENCODE protein complement. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 5495-5500.	7.1	206
2	Insights into the Binding of Phenyltiocarbamide (PTC) Agonist to Its Target Human TAS2R38 Bitter Receptor. PLoS ONE, 2010, 5, e12394.	2.5	97
3	Hypomorphic mutations in POLR3A are a frequent cause of sporadic and recessive spastic ataxia. Brain, 2017, 140, 1561-1578.	7.6	85
4	GOMoDo: A GPCRs Online Modeling and Docking Webserver. PLoS ONE, 2013, 8, e74092.	2.5	84
5	Evidence for a Transient Additional Ligand Binding Site in the TAS2R46 Bitter Taste Receptor. Journal of Chemical Theory and Computation, 2015, 11, 4439-4449.	5.3	70
6	Coarse-Grained/Molecular Mechanics of the TAS2R38 Bitter Taste Receptor: Experimentally-Validated Detailed Structural Prediction of Agonist Binding. PLoS ONE, 2013, 8, e64675.	2.5	67
7	Mutation Analysis of Violaxanthin De-epoxidase Identifies Substrate-binding Sites and Residues Involved in Catalysis. Journal of Biological Chemistry, 2010, 285, 23763-23770.	3.4	59
8	Evaluating the usefulness of protein structure models for molecular replacement. Bioinformatics, 2005, 21, ii72-ii76.	4.1	57
9	Mesencephalic dopaminergic neurons express a repertoire of olfactory receptors and respond to odorant-like molecules. BMC Genomics, 2014, 15, 729.	2.8	46
10	Hybrid Molecular Mechanics/Coarse-Grained Simulations for Structural Prediction of G-Protein Coupled Receptor/Ligand Complexes. PLoS ONE, 2012, 7, e47332.	2.5	45
11	A comprehensive picture of the mutations associated with aromatic amino acid decarboxylase deficiency: from molecular mechanisms to therapy implications. Human Molecular Genetics, 2014, 23, 5429-5440.	2.9	43
12	Siteâ€directed enzymatic PEGylation of the human granulocyte colonyâ€stimulating factor. FEBS Journal, 2009, 276, 6741-6750.	4.7	42
13	Computational design of molecularly imprinted polymer for direct detection of melamine in milk. Separation Science and Technology, 2017, 52, 1441-1453.	2.5	41
14	All muscarinic acetylcholine receptors (M1-M5) are expressed in murine brain microvascular endothelium. Scientific Reports, 2017, 7, 5083.	3.3	40
15	Molecular modeling of ion channels: structural predictions. Current Opinion in Chemical Biology, 2003, 7, 150-156.	6.1	39
16	A Homology Model of the Pore Region of HCN Channels. Biophysical Journal, 2005, 89, 932-944.	0.5	36
17	Agonist Binding to Chemosensory Receptors: A Systematic Bioinformatics Analysis. Frontiers in Molecular Biosciences, 2017, 4, 63.	3.5	36
18	Metal binding affinity and structural properties of calmodulinâ€like protein 14 from Arabidopsis thaliana. Protein Science, 2016, 25, 1461-1471.	7.6	35

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19	Identification of new BMP6 proâ€peptide mutations in patients with iron overload. American Journal of Hematology, 2017, 92, 562-568.	4.1	35
20	Nicotine Blocks the Hyperpolarization-Activated Current Ih and Severely Impairs the Oscillatory Behavior of Oriens-Lacunosum Moleculare Interneurons. Journal of Neuroscience, 2010, 30, 10773-10783.	3.6	34
21	Apparent Mineralocorticoid Excess by a Novel Mutation and Epigenetic Modulation byHSD11B2Promoter Methylation. Journal of Clinical Endocrinology and Metabolism, 2015, 100, E1234-E1241.	3.6	33
22	Predicting ligand binding poses for low-resolution membrane protein models: Perspectives from multiscale simulations. Biochemical and Biophysical Research Communications, 2018, 498, 366-374.	2.1	32
23	Dual binding mode of â€œbitter sugarsâ€•to their human bitter taste receptor target. Scientific Reports, 2019, 9, 8437.	3.3	31
24	A Candidate Ion-Retaining State in the Inward-Facing Conformation of Sodium/Galactose Symporter: Clues from Atomistic Simulations. Journal of Chemical Theory and Computation, 2013, 9, 1240-1246.	5.3	26
25	Genetic and Clinical Heterogeneity in Thirteen New Cases with Aceruloplasminemia. Atypical Anemia as a Clue for an Early Diagnosis. International Journal of Molecular Sciences, 2020, 21, 2374.	4.1	25
26	Structural basis of gating of CNG channels. FEBS Letters, 2005, 579, 1968-1972.	2.8	24
27	Genome-wide Membrane Protein Structure Prediction. Current Genomics, 2013, 14, 324-329.	1.6	24
28	Emergence of a recurrent insertion in the N-terminal domain of the SARS-CoV-2 spike glycoprotein. Virus Research, 2022, 310, 198674.	2.2	24
29	Automatic procedure for using models of proteins in molecular replacement. Proteins: Structure, Function and Bioinformatics, 2006, 66, 689-696.	2.6	23
30	Structural heterogeneity of the Î¼-opioid receptorâ€™s conformational ensemble in the apo state. Scientific Reports, 2017, 7, 45761.	3.3	23
31	Gating in CNGA1 channels. Pflugers Archiv European Journal of Physiology, 2010, 459, 547-555.	2.8	22
32	Identification of novel mutations in hemochromatosis genes by targeted next generation sequencing in Italian patients with unexplained iron overload. American Journal of Hematology, 2016, 91, 420-425.	4.1	22
33	Protein Aggregation and Molecular Crowding. International Review of Cell and Molecular Biology, 2017, 329, 49-77.	3.2	22
34	Loss of the JAK2 intramolecular autoâ€inhibition mechanism is predicted by structural modelling of a novel exon 12 insertion mutation in a case of idiopathic erythrocytosis. British Journal of Haematology, 2008, 142, 986-990.	2.5	21
35	Characterization of C-S Lyase fromC. diphtheriae: A Possible Target for New Antimicrobial Drugs. BioMed Research International, 2013, 2013, 1-13.	1.9	21
36	Genome-wide characterisation and expression profile of the grapevine ATL ubiquitin ligase family reveal biotic and abiotic stress-responsive and development-related members. Scientific Reports, 2016, 6, 38260.	3.3	21

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37	Open Boundary Simulations of Proteins and Their Hydration Shells by Hamiltonian Adaptive Resolution Scheme. Journal of Chemical Theory and Computation, 2017, 13, 5647-5657.	5.3	20
38	Locking CNGA1 Channels in the Open and Closed State. Biophysical Journal, 2006, 90, 3599-3607.	0.5	19
39	Modelling and molecular dynamics of the interaction between the E3 ubiquitin ligase Itch and the E2 UbcH7. Biochemical Pharmacology, 2008, 76, 1620-1627.	4.4	18
40	MERMAID: dedicated web server to prepare and run coarse-grained membrane protein dynamics. Nucleic Acids Research, 2019, 47, W456-W461.	14.5	18
41	Effects of interface mutations on the dimerization of alanine glyoxylate aminotransferase and implications in the mistargeting of the pathogenic variants F152I and I244T. Biochimie, 2016, 131, 137-148.	2.6	17
42	Structure-function relationships of the disease-linked A218T oxytocin receptor variant. Molecular Psychiatry, 2022, 27, 907-917.	7.9	17
43	Structural Requirements for Cooperativity in Ileal Bile Acid-binding Proteins. Journal of Biological Chemistry, 2011, 286, 39307-39317.	3.4	16
44	Evidence of Alternative Splicing as a Regulatory Mechanism for Kissr2 in Pejerrey Fish. Frontiers in Endocrinology, 2018, 9, 604.	3.5	15
45	Structural Prediction of the Dimeric Form of the Mammalian Translocator Membrane Protein TSPO: A Key Target for Brain Diagnostics. International Journal of Molecular Sciences, 2018, 19, 2588.	4.1	15
46	CGMD Platform: Integrated Web Servers for the Preparation, Running, and Analysis of Coarse-Grained Molecular Dynamics Simulations. Molecules, 2020, 25, 5934.	3.8	14
47	The Evaluation of Protein Structure Prediction Results. Molecular Biotechnology, 2008, 39, 1-8.	2.4	13
48	Role of Extracellular Loops and Membrane Lipids for Ligand Recognition in the Neuronal Adenosine Receptor Type 2A: An Enhanced Sampling Simulation Study. Molecules, 2018, 23, 2616.	3.8	13
49	Allosteric sodium binding cavity in GPR3: a novel player in modulation of AÎ² production. Scientific Reports, 2018, 8, 11102.	3.3	13
50	Spinocerebellar ataxia type 14: refining clinicogenetic diagnosis in a rare adultâ€onset disorder. Annals of Clinical and Translational Neurology, 2021, 8, 774-789.	3.7	13
51	The Assessment of Methods for Protein Structure Prediction. , 2008, 413, 43-57.		11
52	Computational molecular biology approaches to ligandâ€target interactions. HFSP Journal, 2009, 3, 228-239.	2.5	11
53	Residues in the Distal Heme Pocket of Arabidopsis Non-Symbiotic Hemoglobins: Implication for Nitrite Reductase Activity. International Journal of Molecular Sciences, 2016, 17, 640.	4.1	11
54	Structural modeling of G-protein coupled receptors: An overview on automatic web-servers. International Journal of Biochemistry and Cell Biology, 2016, 77, 264-274.	2.8	11

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55	Multi-scale simulations of membrane proteins: The case of bitter taste receptors. Journal of Science: Advanced Materials and Devices, 2017, 2, 15-21.	3.1	11
56	Orthosteric and benzodiazepine cavities of the Î±1Î²2Î³2 GABAA receptor: insights from experimentally validated in silico methods. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1597-1615.	3.5	11
57	Effect of the Heteroaromatic Antenna on the Binding of Chiral Eu(III) Complexes to Bovine Serum Albumin. Inorganic Chemistry, 2020, 59, 12564-12577.	4.0	11
58	Robust principal component analysisâ€based prediction of <scp>proteinâ€protein</scp> interaction hot spots. Proteins: Structure, Function and Bioinformatics, 2021, 89, 639-647.	2.6	11
59	Structure/Function Relationships of Phospholipases C Beta. Current Protein and Peptide Science, 2013, 14, 650-657.	1.4	11
60	Transient Interactions of a Cytosolic Protein with Macromolecular and Vesicular Cosolutes: Unspecific and Specific Effects. ChemBioChem, 2015, 16, 2633-2645.	2.6	10
61	GABA_A receptor family: overview on structural characterization. Future Medicinal Chemistry, 2019, 11, 229-245.	2.3	10
62	Role of activeâ€site residues Tyr55 and Tyr114 in catalysis and substrate specificity of Corynebacterium diphtheriae Câ€6 lyase. Proteins: Structure, Function and Bioinformatics, 2015, 83, 78-90.	2.6	9
63	Molecular characterization of HIV-1 Nef and ACOT8 interaction: insights from in silico structural predictions and in vitro functional assays. Scientific Reports, 2016, 6, 22319.	3.3	9
64	MIRATE: MIps RATional dEsign Science Gateway. Journal of Integrative Bioinformatics, 2018, 15, .	1.5	9
65	Multiscale simulations on human Frizzled and Taste2 GPCRs. Current Opinion in Structural Biology, 2019, 55, 8-16.	5.7	9
66	Ligand Pose Predictions for Human G Protein-Coupled Receptors: Insights from the Amber-Based Hybrid Molecular Mechanics/Coarse-Grained Approach. Journal of Chemical Information and Modeling, 2020, 60, 5103-5116.	5.4	9
67	A Mechanistic Model of NMDA and AMPA Receptor-Mediated Synaptic Transmission in Individual Hippocampal CA3-CA1 Synapses: A Computational Multiscale Approach. International Journal of Molecular Sciences, 2021, 22, 1536.	4.1	9
68	Coevolutionary data-based interaction networks approach highlighting key residues across protein families: The case of the G-protein coupled receptors. Computational and Structural Biotechnology Journal, 2020, 18, 1153-1159.	4.1	8
69	Bioinformatics Applications in Life Sciences and Technologies. BioMed Research International, 2016, 2016, 1-2.	1.9	7
70	Unifying view of mechanical and functional hotspots across class A GPCRs. PLoS Computational Biology, 2017, 13, e1005381.	3.2	7
71	Hybrid MM/CG Webserver: Automatic Set Up of Molecular Mechanics/Coarse-Grained Simulations for Human G Protein-Coupled Receptor/Ligand Complexes. Frontiers in Molecular Biosciences, 2020, 7, 576689.	3.5	7
72	Dynamic characterization and substrate binding of cis-2,3-dihydrobiphenyl-2,3-diol dehydrogenaseâ€”an enzyme used in bioremediation. Journal of Molecular Modeling, 2014, 20, 2531.	1.8	6

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73	Identification of aldolase and ferredoxin reductase within the dbt operon of Burkholderia fungorum DBT1. Journal of Basic Microbiology, 2014, 54, 464-469.	3.3	6
74	A Multimodal Approach for Protein Remote Homology Detection. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2015, 12, 1193-1198.	3.0	6
75	Genetic and bioinformatics analysis of four novel <scp>GCK</scp> missense variants detected in Caucasian families with <scp>GCKâ€MODY</scp> phenotype. Clinical Genetics, 2015, 87, 440-447.	2.0	6
76	Impact of Cholesterol on the Stability of Monomeric and Dimeric Forms of the Translocator Protein TSPO: A Molecular Simulation Study. Molecules, 2020, 25, 4299.	3.8	6
77	Molecular Mechanics/Coarse-Grained Models. , 2014, , 165-174.		6
78	NMR Constraints Analyser: a web-server for the graphical analysis of NMR experimental constraints. Nucleic Acids Research, 2010, 38, W628-W632.	14.5	5
79	Conserved charged amino acids are key determinants for fatty acid binding proteins (FABPs)-membrane interactions. A multi-methodological computational approach. Journal of Biomolecular Structure and Dynamics, 2018, 36, 861-877.	3.5	5
80	The Interplay of Cholesterol and Ligand Binding in hTSPO from Classical Molecular Dynamics Simulations. Molecules, 2021, 26, 1250.	3.8	5
81	S-BLOSUM: Classification of 2D Shapes with Biological Sequence Alignment. , 2014, , .		4
82	Structural predictions of neurobiologically relevant G-protein coupled receptors and intrinsically disordered proteins. Archives of Biochemistry and Biophysics, 2015, 582, 91-100.	3.0	4
83	Comprehensive Workflow for the Genome-wide Identification and Expression Meta-analysis of the ATL E3 Ubiquitin Ligase Gene Family in Grapevine. Journal of Visualized Experiments, 2017, , .	0.3	4
84	Chemosensorial G-proteins-Coupled Receptors: A Perspective from Computational Methods. Advances in Experimental Medicine and Biology, 2014, 805, 441-457.	1.6	4
85	Common evolutionary binding mode of rhodopsin-like GPCRs: Insights from structural bioinformatics. AIMS Biophysics, 2017, 4, 543-556.	0.6	4
86	Ligand based conformational space studies of the Î¼-opioid receptor. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129838.	2.4	3
87	A Gain-of-Function Mutation on BCKDK Gene and Its Possible Pathogenic Role in Branched-Chain Amino Acid Metabolism. Genes, 2022, 13, 233.	2.4	3
88	A Novel ALAS2 Missense Mutation in Two Brothers With Iron Overload and Associated Alterations in Serum Hepcidin/Erythroferrone Levels. Frontiers in Physiology, 2020, 11, 581386.	2.8	2
89	A computational strategy to understand structure-activity relationship of 1,3-disubstituted imidazole [1,5-Î±] pyrazine derivatives described as ATP competitive inhibitors of the IGF-1 receptor related to Ewing sarcoma. Journal of Molecular Modeling, 2020, 26, 222.	1.8	2
90	Knowledge Based Membrane Protein Structure Prediction: From X-Ray Crystallography to Bioinformatics and Back to Molecular Biology. , 0, , .		1

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91	Advanced Computational Methods in Molecular Medicine. Journal of Biomedicine and Biotechnology, 2012, 2012, 1-2.	3.0	1
92	Structural bioinformatics: advances and applications. AIP Conference Proceedings, 2006, , .	0.4	0
93	P-D9â€ƒHuman Thioesterase 8 and HIV-1 Nef interaction. Journal of Acquired Immune Deficiency Syndromes (1999), 2014, 67, 90.	2.1	0
94	Gating Mechanism Investigation in Homotetramer CNGA1 Ion Channel by Coarse-Grained Molecular Dynamics Simulation. Biophysical Journal, 2018, 114, 128a.	0.5	0
95	The Two Faces of Bitter Sugars: Insights from Multiscale Simulations. Biophysical Journal, 2019, 116, 478a.	0.5	0
96	Receptors' Mosaics and Allostery for Pharmacology. Biophysical Journal, 2020, 118, 521a-522a.	0.5	0
97	Structural Bioinformatics Approaches to Chemical Senses. IFMBE Proceedings, 2013, , 354-358.	0.3	0
98	Multi-Scale Computational Biology. Biology and Medicine (Aligarh), 2014, 06, .	0.3	0
99	Membrane Proteins: Insights from Computational Biology. Biology and Medicine (Aligarh), 2014, 06, .	0.3	0
100	Identification of New BMP6 Pro-Peptide Mutations in Patients with Unexplained Iron-Overload. Blood, 2016, 128, 264-264.	1.4	0