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	Structure-function relationships of the disease-linked A218T oxytocin receptor variant. Molecular Psychiatry, 2022, 27, 907-917.	7.9	17
2	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
3	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
4	The Interplay of Cholesterol and Ligand Binding in hTSPO from Classical Molecular Dynamics Simulations. Molecules, 2021, 26, 1250.	3.8	5
5	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
6	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
7	Ligand based conformational space studies of the Î¼-opioid receptor. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129838.	2.4	3
8	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
9	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
10	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
11	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
12	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
13	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
14	CGMD Platform: Integrated Web Servers for the Preparation, Running, and Analysis of Coarse-Grained Molecular Dynamics Simulations. Molecules, 2020, 25, 5934.	3.8	14
15	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
16	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
17	Receptors' Mosaics and Allostery for Pharmacology. Biophysical Journal, 2020, 118, 521a-522a.	0.5	0
18	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

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19	MERMAID: dedicated web server to prepare and run coarse-grained membrane protein dynamics. Nucleic Acids Research, 2019, 47, W456-W461.	14.5	18
20	Dual binding mode of â€œbitter sugarsâ€• to their human bitter taste receptor target. Scientific Reports, 2019, 9, 8437.	3.3	31
21	GABA_A receptor family: overview on structural characterization. Future Medicinal Chemistry, 2019, 11, 229-245.	2.3	10
22	Multiscale simulations on human Frizzled and Taste2 GPCRs. Current Opinion in Structural Biology, 2019, 55, 8-16.	5.7	9
23	The Two Faces of Bitter Sugars: Insights from Multiscale Simulations. Biophysical Journal, 2019, 116, 478a.	0.5	0
24	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
25	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
26	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
27	Evidence of Alternative Splicing as a Regulatory Mechanism for Kissr2 in Pejerrey Fish. Frontiers in Endocrinology, 2018, 9, 604.	3.5	15
28	Gating Mechanism Investigation in Homotetramer CNGA1 Ion Channel by Coarse-Grained Molecular Dynamics Simulation. Biophysical Journal, 2018, 114, 128a.	0.5	0
29	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
30	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
31	Allosteric sodium binding cavity in GPR3: a novel player in modulation of AÎ² production. Scientific Reports, 2018, 8, 11102.	3.3	13
32	MIRATE: MIps RATional dEsign Science Gateway. Journal of Integrative Bioinformatics, 2018, 15, .	1.5	9
33	Protein Aggregation and Molecular Crowding. International Review of Cell and Molecular Biology, 2017, 329, 49-77.	3.2	22
34	Computational design of molecularly imprinted polymer for direct detection of melamine in milk. Separation Science and Technology, 2017, 52, 1441-1453.	2.5	41
35	Hypomorphic mutations in POLR3A are a frequent cause of sporadic and recessive spastic ataxia. Brain, 2017, 140, 1561-1578.	7.6	85
36	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

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37	Identification of new BMP6 proâ€peptide mutations in patients with iron overload. American Journal of Hematology, 2017, 92, 562-568.	4.1	35
38	Structural heterogeneity of the Î¼-opioid receptorâ€™s conformational ensemble in the apo state. Scientific Reports, 2017, 7, 45761.	3.3	23
39	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
40	All muscarinic acetylcholine receptors (M1-M5) are expressed in murine brain microvascular endothelium. Scientific Reports, 2017, 7, 5083.	3.3	40
41	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
42	Agonist Binding to Chemosensory Receptors: A Systematic Bioinformatics Analysis. Frontiers in Molecular Biosciences, 2017, 4, 63.	3.5	36
43	Unifying view of mechanical and functional hotspots across class A GPCRs. PLoS Computational Biology, 2017, 13, e1005381.	3.2	7
44	Common evolutionary binding mode of rhodopsin-like GPCRs: Insights from structural bioinformatics. AIMS Biophysics, 2017, 4, 543-556.	0.6	4
45	Bioinformatics Applications in Life Sciences and Technologies. BioMed Research International, 2016, 2016, 1-2.	1.9	7
46	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
47	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
48	Metal binding affinity and structural properties of calmodulinâ€like protein 14 from Arabidopsis thaliana. Protein Science, 2016, 25, 1461-1471.	7.6	35
49	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
50	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
51	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
52	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
53	Identification of New BMP6 Pro-Peptide Mutations in Patients with Unexplained Iron-Overload. Blood, 2016, 128, 264-264.	1.4	0
54	Transient Interactions of a Cytosolic Protein with Macromolecular and Vesicular Cosolutes: Unspecific and Specific Effects. ChemBioChem, 2015, 16, 2633-2645.	2.6	10

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55	A Multimodal Approach for Protein Remote Homology Detection. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2015, 12, 1193-1198.	3.0	6
56	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
57	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
58	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
59	Role of activeâ€site residues Tyr55 and Tyr114 in catalysis and substrate specificity of Corynebacterium diphtheriae Câ€S lyase. Proteins: Structure, Function and Bioinformatics, 2015, 83, 78-90.	2.6	9
60	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
61	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
62	S-BLOSUM: Classification of 2D Shapes with Biological Sequence Alignment. , 2014, , .		4
63	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
64	Mesencephalic dopaminergic neurons express a repertoire of olfactory receptors and respond to odorant-like molecules. BMC Genomics, 2014, 15, 729.	2.8	46
65	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
66	P-D9â€ƒHuman Thioesterase 8 and HIV-1 Nef interaction. Journal of Acquired Immune Deficiency Syndromes (1999), 2014, 67, 90.	2.1	0
67	Chemosensorial G-proteins-Coupled Receptors: A Perspective from Computational Methods. Advances in Experimental Medicine and Biology, 2014, 805, 441-457.	1.6	4
68	Molecular Mechanics/Coarse-Grained Models. , 2014, , 165-174.		6
69	Multi-Scale Computational Biology. Biology and Medicine (Aligarh), 2014, 06, .	0.3	0
70	Membrane Proteins: Insights from Computational Biology. Biology and Medicine (Aligarh), 2014, 06, .	0.3	0
71	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
72	Characterization of C-S Lyase fromC. diphtheriae: A Possible Target for New Antimicrobial Drugs. BioMed Research International, 2013, 2013, 1-13.	1.9	21

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73	Genome-wide Membrane Protein Structure Prediction. Current Genomics, 2013, 14, 324-329.	1.6	24
74	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
75	GOMoDo: A GPCRs Online Modeling and Docking Webserver. PLoS ONE, 2013, 8, e74092.	2.5	84
76	Structure/Function Relationships of Phospholipases C Beta. Current Protein and Peptide Science, 2013, 14, 650-657.	1.4	11
77	Structural Bioinformatics Approaches to Chemical Senses. IFMBE Proceedings, 2013, , 354-358.	0.3	0
78	Advanced Computational Methods in Molecular Medicine. Journal of Biomedicine and Biotechnology, 2012, 2012, 1-2.	3.0	1
79	Hybrid Molecular Mechanics/Coarse-Grained Simulations for Structural Prediction of G-Protein Coupled Receptor/Ligand Complexes. PLoS ONE, 2012, 7, e47332.	2.5	45
80	Structural Requirements for Cooperativity in Ileal Bile Acid-binding Proteins. Journal of Biological Chemistry, 2011, 286, 39307-39317.	3.4	16
81	Gating in CNGA1 channels. Pflugers Archiv European Journal of Physiology, 2010, 459, 547-555.	2.8	22
82	Insights into the Binding of Phenyltiocarbamide (PTC) Agonist to Its Target Human TAS2R38 Bitter Receptor. PLoS ONE, 2010, 5, e12394.	2.5	97
83	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
84	NMR Constraints Analyser: a web-server for the graphical analysis of NMR experimental constraints. Nucleic Acids Research, 2010, 38, W628-W632.	14.5	5
85	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
86	Siteâ€directed enzymatic PEGylation of the human granulocyte colonyâ€stimulating factor. FEBS Journal, 2009, 276, 6741-6750.	4.7	42
87	Computational molecular biology approaches to ligandâ€target interactions. HFSP Journal, 2009, 3, 228-239.	2.5	11
88	The Evaluation of Protein Structure Prediction Results. Molecular Biotechnology, 2008, 39, 1-8.	2.4	13
89	The Assessment of Methods for Protein Structure Prediction. , 2008, 413, 43-57.		11
90	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

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91	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
92	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
93	Locking CNGA1 Channels in the Open and Closed State. Biophysical Journal, 2006, 90, 3599-3607.	0.5	19
94	Automatic procedure for using models of proteins in molecular replacement. Proteins: Structure, Function and Bioinformatics, 2006, 66, 689-696.	2.6	23
95	Structural bioinformatics: advances and applications. AIP Conference Proceedings, 2006, , .	0.4	0
96	Evaluating the usefulness of protein structure models for molecular replacement. Bioinformatics, 2005, 21, ii72-ii76.	4.1	57
97	Structural basis of gating of CNG channels. FEBS Letters, 2005, 579, 1968-1972.	2.8	24
98	A Homology Model of the Pore Region of HCN Channels. Biophysical Journal, 2005, 89, 932-944.	0.5	36
99	Molecular modeling of ion channels: structural predictions. Current Opinion in Chemical Biology, 2003, 7, 150-156.	6.1	39
100	Knowledge Based Membrane Protein Structure Prediction: From X-Ray Crystallography to Bioinformatics and Back to Molecular Biology. , 0, , .		1