Ignacio Fita

List of Publications by Year in descending order

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119 papers	5,594 citations	57719 44 h-index	88593 70 g-index
126 all docs	126 docs citations	126 times ranked	5383 citing authors

#	Article	IF	Citations
1	The active center of catalase. Journal of Molecular Biology, 1985, 185, 21-37.	2.0	404
2	Ca2+ bridges the C2 membrane-binding domain of protein kinase CÎ± directly to phosphatidylserine. EMBO Journal, 1999, 18, 6329-6338.	3.5	323
3	Enzymology and structure of catalases. Advances in Inorganic Chemistry, 2000, 51, 51-106.	0.4	236
4	Structural basis for the high all-trans -retinaldehyde reductase activity of the tumor marker AKR1B10. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 20764-20769.	3.3	172
5	Three-dimensional structure of catalase from Penicillium vitale at 2.0 Ã... resolution. Journal of Molecular Biology, 1986, 188, 49-61.	2.0	160
6	X-ray structure of a minor group human rhinovirus bound to a fragment of its cellular receptor protein. Nature Structural and Molecular Biology, 2004, 11, 429-434.	3.6	143
7	Molecular basis of substrate-induced permeation by an amino acid antiporter. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3935-3940.	3.3	139
8	Structure of Acetylglutamate Kinase, a Key Enzyme for Arginine Biosynthesis and a Prototype for the Amino Acid Kinase Enzyme Family, during Catalysis. Structure, 2002, 10, 329-342.	1.6	126
9	Catalase-peroxidase KatG of Burkholderia pseudomallei at 1.7Ã... resolution. Journal of Molecular Biology, 2003, 327, 475-489.	2.0	126
10	The crystal structure of the complex of PII and acetylglutamate kinase reveals how PII controls the storage of nitrogen as arginine. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 17644-17649.	3.3	113
11	Structure of catalase-A from Saccharomyces cerevisiae. Journal of Molecular Biology, 1999, 286, 135-149.	2.0	106
12	The Structure of Human 4F2hc Ectodomain Provides a Model for Homodimerization and Electrostatic Interaction with Plasma Membrane. Journal of Biological Chemistry, 2007, 282, 31444-31452.	1.6	101
13	The refined structure of beef liver catalase at 2Â·5 Ã... resolution. Acta Crystallographica Section B: Structural Science, 1986, 42, 497-515.	1.8	99
14	Crystal structure of catalase HPII from Escherichia coli. Structure, 1995, 3, 491-502.	1.6	99
15	Structural and mechanistic insights into the association of PKCÎ±-C2 domain to PtdIns(4,5)P ₂. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 6603-6607.	3.3	99
16	Structure of the C2 domain from novel protein kinase CÏµ. A membrane binding model for Ca2+-independent C2 domains. Journal of Molecular Biology, 2001, 311, 837-849.	2.0	97
17	Arginine and nitrogen storage. Current Opinion in Structural Biology, 2008, 18, 673-681.	2.6	92
18	Thirty years of heme catalases structural biology. Archives of Biochemistry and Biophysics, 2012, 525, 102-110.	1.4	90

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19	Comparison of beef liver and Penicillium vitale catalases. Journal of Molecular Biology, 1986, 188, 63-72.	2.0	87
20	Structure and interaction with phospholipids of a prokaryotic lipoxygenase from Pseudomonas aeruginosa. FASEB Journal, 2013, 27, 4811-4821.	0.2	78
21	Retinoic Acid Binds to the C2-Domain of Protein Kinase CÎ±â€. Biochemistry, 2003, 42, 8774-8779.	1.2	76
22	Additional Binding Sites for Anionic Phospholipids and Calcium Ions in the Crystal Structures of Complexes of the C2 Domain of Protein Kinase CÎ±. Journal of Molecular Biology, 2002, 320, 277-291.	2.0	74
23	Crystal Structure of an Archaeal Glycogen Synthase. Journal of Biological Chemistry, 2006, 281, 2923-2931.	1.6	74
24	Aldo-keto reductases from the AKR1B subfamily: Retinoid specificity and control of cellular retinoic acid levels. Chemico-Biological Interactions, 2009, 178, 171-177.	1.7	70
25	Catalase-peroxidases (KatG) Exhibit NADH Oxidase Activity. Journal of Biological Chemistry, 2004, 279, 43098-43106.	1.6	68
26	Essential Role of Proximal Histidine-Asparagine Interaction in Mammalian Peroxidases. Journal of Biological Chemistry, 2009, 284, 25929-25937.	1.6	68
27	Identification of a novel bond between a histidine and the essential tyrosine in catalase HPII of Escherichia coli. Protein Science, 1997, 6, 1016-1023.	3.1	65
28	Structure ofHelicobacter pyloriCatalase, with and without Formic Acid Bound, at 1.6 Ã... Resolutionâ€. Biochemistry, 2004, 43, 3089-3103.	1.2	65
29	Structure of the Heme d of Penicillium vitale and Escherichia coli Catalases. Journal of Biological Chemistry, 1996, 271, 8863-8868.	1.6	64
30	Structure of human carbamoyl phosphate synthetase: deciphering the on/off switch of human ureagenesis. Scientific Reports, 2015, 5, 16950.	1.6	64
31	Structural Bases of Feed-back Control of Arginine Biosynthesis, Revealed by the Structures of Two Hexameric N-Acetylglutamate Kinases, from Thermotoga maritima and Pseudomonas aeruginosa. Journal of Molecular Biology, 2006, 356, 695-713.	2.0	63
32	A Novel Two-domain Architecture Within the Amino Acid Kinase Enzyme Family Revealed by the Crystal Structure of Escherichia coli Glutamate 5-kinase. Journal of Molecular Biology, 2007, 367, 1431-1446.	2.0	62
33	Structure of catalase HPII fromEscherichia coli at 1.9 ï¿½ resolution. , 1999, 34, 155-166.		60
34	The Structures and Electronic Configuration of Compound I Intermediates ofHelicobacterpyloriandPenicillium vitaleCatalases Determined by X-ray Crystallography and QM/MM Density Functional Theory Calculations. Journal of the American Chemical Society, 2007, 129, 4193-4205.	6.6	58
35	L amino acid transporter structure and molecular bases for the asymmetry of substrate interaction. Nature Communications, 2019, 10, 1807.	5.8	57
36	An Electrical Potential in the Access Channel of Catalases Enhances Catalysis. Journal of Biological Chemistry, 2003, 278, 31290-31296.	1.6	56

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37	Isonicotinic Acid Hydrazide Conversion to Isonicotinyl-NAD by Catalase-peroxidases. Journal of Biological Chemistry, 2010, 285, 26662-26673.	1.6	55
38	Theoretical Study of the Mechanisms of Substrate Recognition by Catalase. Journal of the American Chemical Society, 2001, 123, 9665-9672.	6.6	50
39	Substrate flow in catalases deduced from the crystal structures of active site variants of HPII fromEscherichia coli. Proteins: Structure, Function and Bioinformatics, 2001, 44, 270-281.	1.5	50
40	The 1.5 Ã... resolution crystal structure of the carbamate kinase-like carbamoyl phosphate synthetase from the hyperthermophilic archaeon Pyrococcus furiosus , bound to ADP, confirms that this thermostable enzyme is a carbamate kinase, and provides insight into substrate binding and stability in carbamate kinases 1 1Edited by R. Huber. Journal of Molecular Biology, 2000, 299, 463-476.	2.0	49
41	Apo and Holo Structures of an NADP(H)-dependent Cinnamyl Alcohol Dehydrogenase from Saccharomyces cerevisiae. Journal of Molecular Biology, 2004, 341, 1049-1062.	2.0	49
42	Three-dimensional Structure and Enzymatic Function of Proapoptotic Human p53-inducible Quinone Oxidoreductase PIG3. Journal of Biological Chemistry, 2009, 284, 17194-17205.	1.6	48
43	Versatility of the Electronic Structure of Compound I in Catalase-Peroxidases. Journal of the American Chemical Society, 2007, 129, 13436-13446.	6.6	47
44	Carbamate kinase: New structural machinery for making carbamoyl phosphate, the common precursor of pyrimidines and arginine. Protein Science, 1999, 8, 934-940.	3.1	46
45	Structure of the Clade 1 catalase, CatF of Pseudomonas syringae, at 1.8 Ã... resolution. Proteins: Structure, Function and Bioinformatics, 2003, 50, 423-436.	1.5	45
46	A molecular switch and electronic circuit modulate catalase activity in catalaseâ€peroxidases. EMBO Reports, 2005, 6, 1156-1162.	2.0	45
47	Structure of the Dimeric Exonuclease TREX1 in Complex with DNA Displays a Proline-rich Binding Site for WW Domains. Journal of Biological Chemistry, 2007, 282, 14547-14557.	1.6	45
48	Characterization of the Catalase-Peroxidase KatG from Burkholderia pseudomallei by Mass Spectrometry. Journal of Biological Chemistry, 2003, 278, 35687-35692.	1.6	43
49	The Course of Phosphorus in the Reaction of N-Acetyl-l-glutamate Kinase, Determined from the Structures of Crystalline Complexes, Including a Complex with an AlF4â¯ Transition State Mimic. Journal of Molecular Biology, 2003, 331, 231-244.	2.0	40
50	Roles for Arg426 and Trp111 in the Modulation of NADH Oxidase Activity of the Catalase-peroxidase KatG fromBurkholderia pseudomalleiInferred from pH-Induced Structural Changesâ€,â€¡. Biochemistry, 2006, 45, 5171-5179.	1.2	39
51	Structural Characterization of the Ser324Thr Variant of the Catalase-peroxidase (KatG) from Burkholderia pseudomallei. Journal of Molecular Biology, 2005, 345, 21-28.	2.0	34
52	Role of the lateral channel in catalase HPII of Escherichia coli. Protein Science, 1999, 8, 490-498.	3.1	31
53	Mutants That Alter the Covalent Structure of Catalase Hydroperoxidase II from Escherichia coli xs. Journal of Biological Chemistry, 1999, 274, 27717-27725.	1.6	30
54	The mechanism of vault opening from the high resolution structure of the N-terminal repeats of MVP. EMBO Journal, 2009, 28, 3450-3457.	3.5	30

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55	The Carbamoyl-phosphate Synthetase of Pyrococcus furiosus Is Enzymologically and Structurally a Carbamate Kinase. Journal of Biological Chemistry, 1999, 274, 16295-16303.	1.6	29
56	The Proximal Hydrogen-Bonded Residue Controls the Stability of the CompoundIIIIntermediate of Peroxidases and Catalases. Journal of Physical Chemistry B, 2003, 107, 5300-5305.	1.2	29
57	Mycoplasma genitalium adhesin P110 binds sialic-acid human receptors. Nature Communications, 2018, 9, 4471.	5.8	29
58	An Ionizable Active-Site Tryptophan Imparts Catalase Activity to a Peroxidase Core. Journal of the American Chemical Society, 2014, 136, 7249-7252.	6.6	28
59	Structural and biochemical studies of TREX1 inhibition by metals. Identification of a new active histidine conserved in DEDDh exonucleases. Protein Science, 2008, 17, 2059-2069.	3.1	27
60	Binding of the Antitubercular Pro-Drug Isoniazid in the Heme Access Channel of Catalase-Peroxidase (KatG). A Combined Structural and Metadynamics Investigation. Journal of Physical Chemistry B, 2014, 118, 2924-2931.	1.2	27
61	Vibrational Entropy of a Protein: Large Differences between Distinct Conformations. Journal of Chemical Theory and Computation, 2015, 11, 351-359.	2.3	27
62	Minor group human rhinovirusâ€“receptor interactions: Geometry of multimodular attachment and basis of recognition. FEBS Letters, 2009, 583, 235-240.	1.3	26
63	Processivity and Subcellular Localization of Glycogen Synthase Depend on a Non-catalytic High Affinity Glycogen-binding Site. Journal of Biological Chemistry, 2011, 286, 18505-18514.	1.6	25
64	Structural characterization of the NAP; the major adhesion complex of the human pathogen Mycoplasma genitalium. Molecular Microbiology, 2017, 105, 869-879.	1.2	24
65	Two alternative substrate paths for compound I formation and reduction in catalase-peroxidase KatG from Burkholderia pseudomallei. Proteins: Structure, Function and Bioinformatics, 2006, 66, 219-228.	1.5	22
66	Immunodominant proteins P1 and P40/P90 from human pathogen Mycoplasma pneumoniae. Nature Communications, 2020, 11, 5188.	5.8	22
67	Biosynthesis of isoprenoids in plants: Structure of the 2Câ€methylâ€<scp>d</scp>â€erithrytol 2,4â€cyclodiphosphate synthase from Arabidopsis thaliana. Comparison with the bacterial enzymes. Protein Science, 2007, 16, 2082-2088.	3.1	21
68	High Conformational Stability of Secreted Eukaryotic Catalase-peroxidases. Journal of Biological Chemistry, 2012, 287, 32254-32262.	1.6	21
69	Crystal Structure of the Vertebrate NADP(H)-dependent Alcohol Dehydrogenase (ADH8). Journal of Molecular Biology, 2003, 330, 75-85.	2.0	20
70	Substrate Binding and Catalysis in Carbamate Kinase Ascertained by Crystallographic and Site-Directed Mutagenesis Studies: Movements and Significance of a Unique Globular Subdomain of This Key Enzyme for Fermentative ATP Production in Bacteria. Journal of Molecular Biology, 2010, 397, 1261-1275.	2.0	19
71	Vault particles: a new generation of delivery nanodevices. Current Opinion in Biotechnology, 2012, 23, 972-977.	3.3	19
72	Selective photoregulation of the activity of glycogen synthase and glycogen phosphorylase, two key enzymes in glycogen metabolism. Organic and Biomolecular Chemistry, 2015, 13, 7282-7288.	1.5	19

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73	Structure and mechanism of the Nap adhesion complex from the human pathogen Mycoplasma genitalium. Nature Communications, 2020, 11, 2877.	5.8	19
74	Oxygen Binding to Catalase-Peroxidase. Journal of Physical Chemistry Letters, 2011, 2, 196-200.	2.1	18
75	Insight on an Arginine Synthesis Metabolon from the Tetrameric Structure of Yeast Acetylglutamate Kinase. PLoS ONE, 2012, 7, e34734.	1.1	18
76	Spectroscopic and Kinetic Investigation of the Reactions of Peroxyacetic Acid with Burkholderia pseudomallei Catalase-Peroxidase, KatG. Biochemistry, 2013, 52, 7271-7282.	1.2	18
77	Crystallization and preliminary structural analysis of catalase A from Saccharomyces cerevisiae. Protein Science, 1997, 6, 481-483.	3.1	17
78	Characterization of a Large Subunit Catalase Truncated by Proteolytic Cleavageâ€‚â€¡. Biochemistry, 2005, 44, 5597-5605.	1.2	17
79	The dynamic role of distal side residues in heme hydroperoxidase catalysis. Interplay between X-ray crystallography and ab initio MD simulations. Archives of Biochemistry and Biophysics, 2010, 500, 37-44.	1.4	16
80	Structure of the C-terminal domain of the catalaseâ€“peroxidase KatG fromEscherichia coli. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 1824-1832.	2.5	15
81	Two Crystal Structures of Escherichia coli N-Acetyl-l-Glutamate Kinase Demonstrate the Cycling between Open and Closed Conformations. Journal of Molecular Biology, 2010, 399, 476-490.	2.0	15
82	Electronic State of the Molecular Oxygen Released by Catalase. Journal of Physical Chemistry A, 2008, 112, 12842-12848.	1.1	14
83	Modulation of Heme Orientation and Binding by a Single Residue in Catalase HPII of Escherichia coli. Biochemistry, 2011, 50, 2101-2110.	1.2	14
84	The <scp>EAGR</scp> box structure: a motif involved in mycoplasma motility. Molecular Microbiology, 2012, 86, 382-393.	1.2	14
85	Lyase activity of glycogen synthase: Is an elimination/addition mechanism a possible reaction pathway for retaining glycosyltransferases?. IUBMB Life, 2012, 64, 649-658.	1.5	14
86	Reâ€engineering specificity in 1,3â€1, 4â€Î²â€glucanase to accept branched xyloglucan substrates. Proteins: Structure, Function and Bioinformatics, 2011, 79, 365-375.	1.5	12
87	Influence of main channel structure on H2O2 access to the heme cavity of catalase KatE of Escherichia coli. Archives of Biochemistry and Biophysics, 2012, 526, 54-59.	1.4	12
88	New features of vault architecture and dynamics revealed by novel refinement using the deformable elastic network approach. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 1054-1061.	2.5	12
89	A first principles study of the binding of formic acid in catalase complementing high resolution X-ray structures. Chemical Physics, 2006, 323, 129-137.	0.9	11
90	The Catalase Activity of Catalase-Peroxidases Is Modulated by Changes in the pK_a of the Distal Histidine. Biochemistry, 2017, 56, 2271-2281.	1.2	11

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91	Prediction of Protein Configurational Entropy (Popcoen). Journal of Chemical Theory and Computation, 2018, 14, 1811-1819.	2.3	11
92	N-Acetyl-L-glutamate kinase from Escherichia coli: cloning of the gene, purification and crystallization of the recombinant enzyme and preliminary X-ray analysis of the free and ligand-bound forms. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 1350-1352.	2.5	10
93	Structural Asymmetry and Disulfide Bridges among Subunits Modulate the Activity of Human Malonyl-CoA Decarboxylase*. Journal of Biological Chemistry, 2013, 288, 11907-11919.	1.6	10
94	Calcineurin Undergoes a Conformational Switch Evoked via Peptidyl-Prolyl Isomerization. PLoS ONE, 2015, 10, e0134569.	1.1	10
95	KatG-Mediated Oxidation Leading to Reduced Susceptibility of Bacteria to Kanamycin. ACS Omega, 2018, 3, 4213-4219.	1.6	10
96	Combining experimental data for structure determination of flexible multimeric macromolecules by molecular replacement. Acta Crystallographica Section D: Biological Crystallography, 2006, 62, 467-475.	2.5	9
97	Crystal Structure of Brucella abortus Deoxyxylulose-5-phosphate Reductoisomerase-like (DRL) Enzyme Involved in Isoprenoid Biosynthesis. Journal of Biological Chemistry, 2012, 287, 15803-15809.	1.6	9
98	Representation of noncovalent interactions in protein structures. Journal of Molecular Graphics, 1992, 10, 96-100.	1.7	8
99	Structure of glycerol-3-phosphate dehydrogenase (GPD1) fromSaccharomyces cerevisiaeat 2.45â€…Ã… resolution. Acta Crystallographica Section F: Structural Biology Communications, 2012, 68, 1279-1283.	0.7	8
100	A Major Determinant for Gliding Motility in Mycoplasma genitalium. Journal of Biological Chemistry, 2015, 290, 1699-1711.	1.6	8
101	Inhibitory properties of 1,4-dideoxy-1,4-imino-<scp>d</scp>-arabinitol (DAB) derivatives acting on glycogen metabolising enzymes. Organic and Biomolecular Chemistry, 2016, 14, 9105-9113.	1.5	8
102	The nucleotideâ€bound/substrateâ€bound conformation of the Mycoplasma genitalium DnaK chaperone. Protein Science, 2018, 27, 1000-1007.	3.1	8
103	Crystallization and preliminary X-ray diffraction analysis of catalase HPII from Escherichia coli. Journal of Molecular Biology, 1990, 213, 219-220.	2.0	7
104	Crystallization and preliminary X-ray analysis of the catalaseâ€“peroxidase KatG fromBurkholderia pseudomallei. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 2184-2186.	2.5	7
105	Crystallization and preliminary X-ray analysis of clade I catalases fromPseudomonas syringaeandListeria seeligeri. Acta Crystallographica Section D: Biological Crystallography, 2001, 57, 1184-1186.	2.5	6
106	Testing the mutual information expansion of entropy with multivariate Gaussian distributions. Journal of Chemical Physics, 2017, 147, 224102.	1.2	6
107	Cisâ€trans proline isomers in the catalytic domain of calcineurin. FEBS Journal, 2019, 286, 1230-1239.	2.2	6
108	Crystallization and preliminary X-ray analysis of the hydroperoxidase I C-terminal domain fromEscherichia coli. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 853-855.	2.5	5

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109	Structure ofPisum sativumRubisco with bound ribulose 1,5-bisphosphate. Acta Crystallographica Section F: Structural Biology Communications, 2013, 69, 10-14.	0.7	5
110	Structure-Guided Mutations in the Terminal Organelle Protein MG491 Cause Major Motility and Morphologic Alterations on Mycoplasma genitalium. PLoS Pathogens, 2016, 12, e1005533.	2.1	5
111	Structural Insights into Subunits Assembly and the Oxyester Splicing Mechanism of Neq pol Split Intein. Cell Chemical Biology, 2018, 25, 871-879.e2.	2.5	5
112	Preliminary analysis of two and three dimensional crystals of vault ribonucleoprotein particles. Journal of Structural Biology, 2005, 151, 111-115.	1.3	4
113	Theory Uncovers the Role of the Methionineâ€“Tyrosineâ€“Tryptophan Radical Adduct in the Catalase Reaction of KatGs: O₂â€‰Release Mediated by Protonâ€Coupled Electron Transfer. Chemistry - A European Journal, 2018, 24, 5388-5395.	1.7	4
114	Eukaryotic Catalase-Peroxidase: The Role of the Trp-Tyr-Met Adduct in Protein Stability, Substrate Accessibility, and Catalysis of Hydrogen Peroxide Dismutation. Biochemistry, 2015, 54, 5425-5438.	1.2	3
115	Crystallization and preliminary structural results of catalase from human erythrocytes. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 1066-1068.	2.5	2
116	Thermal motion in proteins: Large effects on the time-averaged interaction energies. AIP Advances, 2016, 6, 035020.	0.6	2
117	Alternative conformation of the C-domain of the P140 protein from Mycoplasma genitalium. Acta Crystallographica Section F, Structural Biology Communications, 2020, 76, 508-516.	0.4	2
118	Entropic Stabilization of Cas4 Protein SSO0001 Predicted with Popcoen. Entropy, 2018, 20, 580.	1.1	1
119	Tumor mesenquimÃ¡tico fosfatÃºrico de pelvis: abordaje multidisciplinario. Revista De La AsociaciÃ³n Argentina De Ortopedia Y TraumatologÃa, 2022, 87, 360-370.	0.0	1