

# Fernando Danilo González Nilo

## List of Publications by Year in descending order

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155  
papers

3,333  
citations

159358

30  
h-index

197535

49  
g-index

155  
all docs

155  
docs citations

155  
times ranked

4972  
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular Determinants of BK Channel Functional Diversity and Functioning. <i>Physiological Reviews</i> , 2017, 97, 39-87.	13.1	213
2	Dissection of the components for PIP2 activation and thermosensation in TRP channels. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 10246-10251.	3.3	192
3	Intracellular trafficking and cellular uptake mechanism of PHBV nanoparticles for targeted delivery in epithelial cell lines. <i>Journal of Nanobiotechnology</i> , 2017, 15, 1.	4.2	115
4	Neutralization of a single arginine residue gates open a two-pore domain, alkali-activated K <sup>+</sup> channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 666-671.	3.3	106
5	Paclitaxel-PHBV nanoparticles and their toxicity to endometrial and primary ovarian cancer cells. <i>Biomaterials</i> , 2013, 34, 4098-4108.	5.7	87
6	LprG-Mediated Surface Expression of Lipoarabinomannan Is Essential for Virulence of <i>Mycobacterium tuberculosis</i> . <i>PLoS Pathogens</i> , 2014, 10, e1004376.	2.1	82
7	Computationally Efficient Methodology for Atomic-Level Characterization of Dendrimer-Drug Complexes: A Comparison of Amine- and Acetyl-Terminated PAMAM. <i>Journal of Physical Chemistry B</i> , 2013, 117, 6801-6813.	1.2	80
8	Thermally activated TRP channels: molecular sensors for temperature detection. <i>Physical Biology</i> , 2018, 15, 021001.	0.8	80
9	Structure and application of antifreeze proteins from Antarctic bacteria. <i>Microbial Cell Factories</i> , 2017, 16, 138.	1.9	70
10	Molecular Determinants of Phosphatidylinositol 4,5-Bisphosphate (PI(4,5)P <sub>2</sub> ) Binding to Transient Receptor Potential V1 (TRPV1) Channels. <i>Journal of Biological Chemistry</i> , 2015, 290, 2086-2098.	1.6	65
11	Calculating Position-Dependent Diffusivity in Biased Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 876-882.	2.3	64
12	Photophysics and photochemistry of dyes bound to human serum albumin are determined by the dye localization. <i>Photochemical and Photobiological Sciences</i> , 2010, 9, 93-102.	1.6	61
13	Study of Interaction Energies between the PAMAM Dendrimer and Nonsteroidal Anti-Inflammatory Drug Using a Distributed Computational Strategy and Experimental Analysis by ESI-MS/MS. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2031-2039.	1.2	59
14	Insights into the Structural Basis of N2 and O6 Substituted Guanine Derivatives as Cyclin-Dependent Kinase 2 (CDK2) Inhibitors: Prediction of the Binding Modes and Potency of the inhibitors by Docking and ONIOM Calculations. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 886-899.	2.5	57
15	Development of a nanoparticle-based oral vaccine for Atlantic salmon against ISAV using an alphavirus replicon as adjuvant. <i>Fish and Shellfish Immunology</i> , 2015, 45, 157-166.	1.6	54
16	Structural determinants of 5 $\alpha$ - $\Delta^2,6\alpha$ -epoxyeicosatrienoic acid binding to and activation of TRPV4 channel. <i>Scientific Reports</i> , 2017, 7, 10522.	1.6	53
17	Engineering Atrazine Loaded Poly (lactic-co-glycolic Acid) Nanoparticles to Ameliorate Environmental Challenges. <i>Journal of Agricultural and Food Chemistry</i> , 2018, 66, 7889-7898.	2.4	47
18	Structure-antioxidant activity relationships of flavonoids isolated from the resinous exudate of <i>Heliotropium sinuatum</i> . <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 309-312.	1.0	45

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19	Shared and Group-Specific Features of the Rotavirus RNA Polymerase Reveal Potential Determinants of Gene Reassortment Restriction. <i>Journal of Virology</i> , 2009, 83, 6135-6148.	1.5	45
20	Synthesis, Biological Evaluation, and Molecular Simulation of Chalcones and Aurones as Selective MAO-B Inhibitors. <i>Chemical Biology and Drug Design</i> , 2015, 85, 685-695.	1.5	45
21	Histidine Triad-like Motif of the Rotavirus NSP2 Octamer Mediates both RTPase and NTPase Activities. <i>Journal of Molecular Biology</i> , 2006, 362, 539-554.	2.0	44
22	Intrinsic Electrostatic Potential in the BK Channel Pore: Role in Determining Single Channel Conductance and Block. <i>Journal of General Physiology</i> , 2008, 131, 147-161.	0.9	39
23	Distinct roles of the last transmembrane domain in controlling <i>Arabidopsis</i> K <sup>+</sup> channel activity. <i>New Phytologist</i> , 2009, 182, 380-391.	3.5	38
24	Role of the Histidine Triad-like Motif in Nucleotide Hydrolysis by the Rotavirus RNA-packaging Protein NSP2. <i>Journal of Biological Chemistry</i> , 2004, 279, 10624-10633.	1.6	36
25	Quantitative Structure-Activity Relationship of Rubiscolin Analogues as $\mu$ Opioid Peptides Using Comparative Molecular Field Analysis (CoMFA) and Comparative Molecular Similarity Indices Analysis (CoMSIA). <i>Journal of Agricultural and Food Chemistry</i> , 2007, 55, 8101-8104.	2.4	36
26	Location of TEMPO derivatives in micelles: subtle effect of the probe orientation. <i>Food Chemistry</i> , 2016, 192, 395-401.	4.2	35
27	Excessive release of inorganic polyphosphate by ALS/FTD astrocytes causes non-cell-autonomous toxicity to motoneurons. <i>Neuron</i> , 2022, 110, 1656-1670.e12.	3.8	33
28	Solute-Solvent Interactions of Flavonoids in Organic Solvents. <i>Journal of Solution Chemistry</i> , 2003, 32, 781-790.	0.6	32
29	Structural requirements of pyrido[2,3-d]pyrimidin-7-one as CDK4/D inhibitors: 2D autocorrelation, CoMFA and CoMSIA analyses. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 6103-6115.	1.4	32
30	Supramolecular complexes of quantum dots and a polyamidoamine (PAMAM)-folate derivative for molecular imaging of cancer cells. <i>Analytical and Bioanalytical Chemistry</i> , 2011, 400, 483-492.	1.9	32
31	Gating of a pH-Sensitive K <sub>2</sub> P Potassium Channel by an Electrostatic Effect of Basic Sensor Residues on the Selectivity Filter. <i>PLoS ONE</i> , 2011, 6, e16141.	1.1	32
32	Docking and Quantitative Structure-Activity Relationship Studies for the Bisphenylbenzimidazole Family of Non-Nucleoside Inhibitors of HIV-1 Reverse Transcriptase. <i>Chemical Biology and Drug Design</i> , 2008, 72, 360-369.	1.5	30
33	Study of the Interaction between Progesterone and $\beta$ -Cyclodextrin by Electrochemical Techniques and Steered Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2008, 112, 10194-10201.	1.2	30
34	Self-Assembly of Amphiphilic Dendrimers: The Role of Generation and Alkyl Chain Length in siRNA Interaction. <i>Scientific Reports</i> , 2016, 6, 29436.	1.6	30
35	2D Autocorrelation, CoMFA, and CoMSIA modeling of protein tyrosine kinases' inhibition by substituted pyrido[2,3-d]pyrimidine derivatives. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 810-821.	1.4	29
36	Insight into the Properties of Cardiolipin Containing Bilayers from Molecular Dynamics Simulations, Using a Hybrid All-Atom/United-Atom Force Field. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1765-1773.	2.3	29

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37	The complex of PAMAM-OH dendrimer with Angiotensin (1&ndash;7) prevented the disuse-induced skeletal muscle atrophy in mice. <i>International Journal of Nanomedicine</i> , 2017, Volume 12, 1985-1999.	3.3	29
38	Pore dimensions and the role of occupancy in unitary conductance of Shaker K channels. <i>Journal of General Physiology</i> , 2015, 146, 133-146.	0.9	28
39	Experimental and theoretical binding affinity between polyvinylpyrrolidone and selected phenolic compounds from food matrices. <i>Food Chemistry</i> , 2015, 168, 464-470.	4.2	28
40	In Silico Study of Coumarins and Quinolines Derivatives as Potent Inhibitors of SARS-CoV-2 Main Protease. <i>Frontiers in Chemistry</i> , 2020, 8, 595097.	1.8	28
41	Nanoinformatics: an emerging area of information technology at the intersection of bioinformatics, computational chemistry and nanobiotechnology. <i>Biological Research</i> , 2011, 44, 43-51.	1.5	27
42	Integration of target discovery, drug discovery and drug delivery: A review on computational strategies. <i>Wiley Interdisciplinary Reviews: Nanomedicine and Nanobiotechnology</i> , 2019, 11, e1554.	3.3	27
43	Docking and Molecular Dynamics of Steviol Glycosideâ€“Human Bitter Receptor Interactions. <i>Journal of Agricultural and Food Chemistry</i> , 2016, 64, 7585-7596.	2.4	26
44	Anionic Carbosilane Dendrimers Destabilize the GP120-CD4 Complex Blocking HIV-1 Entry and Cell to Cell Fusion. <i>Bioconjugate Chemistry</i> , 2018, 29, 1584-1594.	1.8	26
45	Effect of Terminal Groups of Dendrimers in the Complexation with Antisense Oligonucleotides and Cell Uptake. <i>Nanoscale Research Letters</i> , 2016, 11, 66.	3.1	24
46	Biosynthesis of Methoxypyrazines: Elucidating the Structural/Functional Relationship of Two <i>Vitis vinifera</i> <i>O</i>-Methyltransferases Capable of Catalyzing the Putative Final Step of the Biosynthesis of 3-Alkyl-2-Methoxypyrazine.. <i>Journal of Agricultural and Food Chemistry</i> , 2011, 59, 7310-7316.	2.4	23
47	Molecular Basis of Drug Resistance in A/H1N1 Virus. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 2650-2656.	2.5	23
48	Mutation Arg336 to Lys in <i>Saccharomyces cerevisiae</i> phosphoenolpyruvate carboxykinase originates an enzyme with increased oxaloacetate decarboxylase activity. <i>FEBS Letters</i> , 2001, 493, 1-5.	1.3	22
49	Gating of two-pore domain K <sup>+</sup> channels by extracellular pH. <i>Biochemical Society Transactions</i> , 2006, 34, 899-902.	1.6	22
50	Dielectric and dynamic-mechanical study of the mobility of poly(t-butylacrylate) chains in diblock copolymers: Polystyrene-b-poly(t-butylacrylate). <i>Polymer</i> , 2008, 49, 5650-5658.	1.8	22
51	Biotransformation of 2,4,6-Trinitrotoluene by <i>Pseudomonas</i> sp. TNT3 isolated from Deception Island, Antarctica. <i>Environmental Pollution</i> , 2020, 262, 113922.	3.7	22
52	<i>Penicillium purpurogenum</i> produces two GH family 43 enzymes with Î²-xylosidase activity, one monofunctional and the other bifunctional: Biochemical and structural analyses explain the difference. <i>Archives of Biochemistry and Biophysics</i> , 2013, 540, 117-124.	1.4	21
53	Interaction between the Linker, Pre-S1, and TRP Domains Determines Folding, Assembly, and Trafficking of TRPV Channels. <i>Structure</i> , 2015, 23, 1404-1413.	1.6	21
54	A folding reaction at the C-terminal domain drives temperature sensing in TRPM8 channels. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 20298-20304.	3.3	21

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55	Distributed Structures Underlie Gating Differences between the Kin Channel KAT1 and the Kout Channel SKOR. <i>Molecular Plant</i> , 2010, 3, 236-245.	3.9	20
56	The pH sensor of the plant K <sup>+</sup> -uptake channel KAT1 is built from a sensory cloud rather than from single key amino acids. <i>Biochemical Journal</i> , 2012, 442, 57-63.	1.7	20
57	Effective pore size and radius of capture for K <sup>+</sup> ions in K-channels. <i>Scientific Reports</i> , 2016, 6, 19893.	1.6	19
58	Stretch-Induced Activation of Pannexin 1 Channels Can Be Prevented by PKA-Dependent Phosphorylation. <i>International Journal of Molecular Sciences</i> , 2020, 21, 9180.	1.8	19
59	Hydrophobic interaction between contiguous residues in the S6 transmembrane segment acts as a stimuli integration node in the BK channel. <i>Journal of General Physiology</i> , 2015, 145, 61-74.	0.9	18
60	Structure-Driven Pharmacology of Transient Receptor Potential Channel Vanilloid 1. <i>Molecular Pharmacology</i> , 2016, 90, 300-308.	1.0	18
61	Structural determinants of TRPV4 inhibition and identification of new antagonists with antiviral activity. <i>British Journal of Pharmacology</i> , 2020, , .	2.7	17
62	Theobroma cacao L. compounds: Theoretical study and molecular modeling as inhibitors of main SARS-CoV-2 protease. <i>Biomedicine and Pharmacotherapy</i> , 2021, 140, 111764.	2.5	17
63	Endogenous pannexin1 channels form functional intercellular cell-cell channels with characteristic voltage-dependent properties. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2202104119.	3.3	17
64	Lysine 213 and Histidine 233 Participate in Mn(II) Binding and Catalysis in <i>Saccharomyces cerevisiae</i> Phosphoenolpyruvate Carboxykinase. <i>Biochemistry</i> , 2002, 41, 12763-12770.	1.2	16
65	A computational ONIOM model for the description of the H-bond interactions between NU2058 analogues and CDK2 active site. <i>Chemical Physics Letters</i> , 2009, 479, 149-155.	1.2	16
66	Hydrogen peroxide and hypochlorous acid influx through the major <i>S. Typhimurium</i> porin OmpD is affected by substitution of key residues of the channel. <i>Archives of Biochemistry and Biophysics</i> , 2015, 568, 38-45.	1.4	16
67	Mechanistic Studies on the Self-Assembly of PLGA Patchy Particles and Their Potential Applications in Biomedical Imaging. <i>Langmuir</i> , 2016, 32, 7929-7942.	1.6	16
68	A physiologic rise in cytoplasmic calcium ion signal increases pannexin1 channel activity via a C-terminus phosphorylation by CaMKII. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, e2108967118.	3.3	16
69	Nanoinformatics: developing new computing applications for nanomedicine. <i>Computing (Vienna/New)</i> Tj ETQq1 1 0.784314 15 /Over	3.2	15
70	Block copolymers in the synthesis of gold nanoparticles. Two new approaches: Copolymer aggregates as reductants and stabilizers and simultaneous formation of copolymer aggregates and gold nanoparticles. <i>Journal of Polymer Science Part A</i> , 2014, 52, 3069-3079.	2.5	15
71	Identification and Functional Expression of a Glutamate- and Avermectin-Gated Chloride Channel from <i>Caligus rogercresseyi</i> , a Southern Hemisphere Sea Louse Affecting Farmed Fish. <i>PLoS Pathogens</i> , 2014, 10, e1004402.	2.1	14
72	PAMAM G4 dendrimers as inhibitors of the iron storage properties of human L-chain ferritin. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 19001-19011.	1.3	14

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73	Î²1-subunit-induced structural rearrangements of the Ca <sup>2+</sup> - and voltage-activated K <sup>+</sup> (BK) channel. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E3231-9.	3.3	14
74	The molecular nature of the 17Î²-Estradiol binding site in the voltage- and Ca <sup>2+</sup> -activated K <sup>+</sup> (BK) channel Î²1 subunit. Scientific Reports, 2019, 9, 9965.	1.6	14
75	Biomimetics: From Bioinformatics to Rational Design of Dendrimers as Gene Carriers. PLoS ONE, 2015, 10, e0138392.	1.1	14
76	The crystal structure of ferritin from Chlorobium tepidum reveals a new conformation of the 4-fold channel for this protein family. Biochimie, 2014, 106, 39-47.	1.3	13
77	Evaluation by site-directed mutagenesis of active site amino acid residues of Anaerobiospirillum succiniciproducens phosphoenolpyruvate carboxykinase. The Protein Journal, 2002, 21, 393-400.	1.1	12
78	Mechanism of voltage sensing in Ca <sup>2+</sup> - and voltage-activated K <sup>+</sup> (BK) channels. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	12
79	Surface characterization and study of Langmuir films of poly(4-vinylpyridine) quaternized withn-alkylbromide. Polymer International, 2001, 50, 858-862.	1.6	11
80	Ligand interactions and protein conformational changes of phosphopyridoxyl-labeled Escherichia coli phosphoenolpyruvate carboxykinase determined by fluorescence spectroscopy. FEBS Journal, 2002, 269, 4960-4968.	0.2	11
81	Site-directed mutagenesis study of the microenvironment characteristics of Lys213 of Saccharomyces cerevisiae phosphoenolpyruvate carboxykinase. Biochimie, 2006, 88, 663-672.	1.3	11
82	Selecting optimal mixtures of natural sweeteners for carbonated soft drinks through multi-objective decision modeling and sensory validation. Journal of Sensory Studies, 2018, 33, e12466.	0.8	11
83	Experimental and Computational Characterization of the Interaction between Gold Nanoparticles and Polyamidoamine Dendrimers. Langmuir, 2018, 34, 10063-10072.	1.6	11
84	The Collaboratory for Structural Nanobiology. Biophysical Journal, 2009, 96, 49a.	0.2	10
85	In Silico Analysis of Putative Paralytic Shellfish Poisoning Toxins Export Proteins in Cyanobacteria. PLoS ONE, 2013, 8, e55664.	1.1	10
86	Synthesis and characterization of an insoluble polymer based on polyamidoamine: Applications for the decontamination of metals in aqueous systems. Journal of Environmental Management, 2015, 147, 321-329.	3.8	10
87	Structural analysis of binding functionality of folic acid-PEG dendrimers against folate receptor. Journal of Molecular Graphics and Modelling, 2017, 72, 201-208.	1.3	10
88	Increasing the intracellular isoprenoid pool in Saccharomyces cerevisiae by structural fine-tuning of a bifunctional farnesyl diphosphate synthase. FEMS Yeast Research, 2017, 17, .	1.1	10
89	Cationic Carbosilane Dendritic Systems as Promising Anti-Amyloid Agents in Type 2 Diabetes. Chemistry - A European Journal, 2020, 26, 7609-7621.	1.7	10
90	Nucleotide specificity of Saccharomyces cerevisiae phosphoenolpyruvate carboxykinase Kinetics, fluorescence spectroscopy, and molecular simulation studies. International Journal of Biochemistry and Cell Biology, 2006, 38, 576-588.	1.2	9

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91	Molecular dynamics simulation of the aqueous solvation shell of cellulose and xanthate ester derivatives. <i>Journal of Physical Organic Chemistry</i> , 2006, 19, 896-901.	0.9	9
92	K <sup>+</sup> Conduction and Mg <sup>2+</sup> Blockade in a Shaker Kv-Channel Single Point Mutant with an Unusually High Conductance. <i>Biophysical Journal</i> , 2012, 103, 1198-1207.	0.2	9
93	Protein Function in Extremely Acidic Conditions: Molecular Simulations of a Predicted Aquaporin and a Potassium Channel in <i>Acidithiobacillus Ferrooxidans</i> . <i>Advanced Materials Research</i> , 0, 71-73, 211-214.	0.3	8
94	pH-dependent nano-capturing of tartaric acid using dendrimers. <i>Soft Matter</i> , 2014, 10, 600-608.	1.2	8
95	Effect of Several HIV Antigens Simultaneously Loaded with G2-NN16 Carbosilane Dendrimer in the Cell Uptake and Functionality of Human Dendritic Cells. <i>Bioconjugate Chemistry</i> , 2016, 27, 2844-2849.	1.8	8
96	Self-Assembly Behavior of Amphiphilic Janus Dendrimers in Water: A Combined Experimental and Coarse-Grained Molecular Dynamics Simulation Approach. <i>Molecules</i> , 2018, 23, 969.	1.7	8
97	Novel TRPV1 Channel Agonists With Faster and More Potent Analgesic Properties Than Capsaicin. <i>Frontiers in Pharmacology</i> , 2020, 11, 1040.	1.6	8
98	Different Classes of Antidepressants Inhibit the Rat $\alpha 7$ Nicotinic Acetylcholine Receptor by Interacting within the Ion Channel: A Functional and Structural Study. <i>Molecules</i> , 2021, 26, 998.	1.7	8
99	Dynamic Mechanical and Dielectric Relaxational Behavior of Poly(cyclohexylalkyl methacrylate)s. <i>Macromolecules</i> , 2001, 34, 6312-6317.	2.2	7
100	<i>Saccharomyces cerevisiae</i> phosphoenolpyruvate carboxykinase: theoretical and experimental study of the effect of glutamic acid 284 on the protonation state of lysine 213. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2002, 1599, 65-71.	1.1	7
101	Substrate binding to fluorescent labeled wild type, Lys213Arg, and His233Gln <i>Saccharomyces cerevisiae</i> phosphoenolpyruvate carboxykinases. <i>International Journal of Biochemistry and Cell Biology</i> , 2004, 36, 861-869.	1.2	7
102	<i>Anaerobiospirillum succiniciproducens</i> phosphoenolpyruvate carboxykinase. Mutagenesis at metal site 1. <i>Biochimie</i> , 2004, 86, 47-51.	1.3	7
103	Role of electrostatics on membrane binding, aggregation and destabilization induced by NAD(P)H dehydrogenases. Implication in membrane fusion. <i>Biophysical Chemistry</i> , 2008, 137, 126-132.	1.5	7
104	Inclusion complexes containing poly( $\epsilon$ -caprolactone)diol and cyclodextrins. Experimental and theoretical studies. <i>Polymer</i> , 2009, 50, 2926-2932.	1.8	7
105	Site-directed mutations and kinetic studies show key residues involved in alkylammonium interactions and reveal two sites for phosphorylcholine in <i>Pseudomonas aeruginosa</i> phosphorylcholine phosphatase. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011, 1814, 858-863.	1.1	7
106	Nano-Detoxification of Organophosphate Agents by PAMAM Derivatives. <i>Journal of the Brazilian Chemical Society</i> , 2015, , .	0.6	7
107	Inorganic polyphosphate as an energy source in tumorigenesis. <i>Oncotarget</i> , 2020, 11, 4613-4624.	0.8	7
108	Urea-induced unfolding studies of free- and ligand-bound tetrameric ATP-dependent <i>Saccharomyces cerevisiae</i> phosphoenolpyruvate carboxykinase. <i>International Journal of Biochemistry and Cell Biology</i> , 2002, 34, 645-656.	1.2	6



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109	Relevance of phenylalanine 216 in the affinity of <i>Saccharomyces cerevisiae</i> phosphoenolpyruvate carboxykinase for Mn(II). <i>Protein Journal</i> , 2007, 26, 135-141.	0.7	6
110	The C-Terminal Regions Have an Important Role in the Activity of the Ferroxidase Center and the Stability of <i>Chlorobium tepidum</i> Ferritin. <i>Protein Journal</i> , 2014, 33, 211-220.	0.7	6
111	Photophysical studies of the interactions of poly(amidoamine) generation zero (PAMAM G0) with copper and zinc ions. <i>Journal of Luminescence</i> , 2015, 164, 23-30.	1.5	6
112	Multiscale Molecular Simulations Applied to Nucleic Acid-Dendrimer Interactions Studies. <i>Current Pharmaceutical Design</i> , 2017, 23, 3062-3075.	0.9	6
113	<i>Anaerobiospirillum succiniciproducens</i> Phosphoenolpyruvate Carboxykinase: Mutagenesis at Metal Site 2. <i>The Protein Journal</i> , 2003, 22, 515-519.	1.1	5
114	In-Silico Nanobio-Design. A New Frontier in Computational Biology. <i>Current Topics in Medicinal Chemistry</i> , 2007, 7, 1537-1540.	1.0	5
115	A CoMSIA study on the adenosine kinase inhibition of pyrrolo[2,3-d]pyrimidine nucleoside analogues. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 5103-5108.	1.4	5
116	Molecular modeling of the complexes between <i>Saccharomyces cerevisiae</i> phosphoenolpyruvate carboxykinase and the ATP analogs pyridoxal 5'-diphosphoadenosine and pyridoxal 5'-triphosphoadenosine. Specific labeling of lysine 290. <i>The Protein Journal</i> , 2000, 19, 67-73.	1.1	4
117	Surface characterization of poly(4-vinylpyridine) quaternized with tetradecyl bromide: effect of the degree of quaternization. <i>Journal of Colloid and Interface Science</i> , 2004, 271, 181-186.	5.0	4
118	Relevance of Arg457 for the nucleotide affinity of <i>Saccharomyces cerevisiae</i> phosphoenolpyruvate carboxykinase. <i>International Journal of Biochemistry and Cell Biology</i> , 2008, 40, 1883-1889.	1.2	4
119	<i>Penicillium purpurogenum</i> produces a novel endo-1,5-arabinanase, active on debranched arabinan, short arabinooligosaccharides and on the artificial substrate p-nitrophenyl arabinofuranoside. <i>Carbohydrate Research</i> , 2018, 455, 106-113.	1.1	4
120	Thermodynamic and structural basis of temperature-dependent gating in TRP channels. <i>Biochemical Society Transactions</i> , 2021, 49, 2211-2219.	1.6	4
121	A theoretical study on the basicity of carbonyl compounds in CCl <sub>4</sub> . <i>Tetrahedron</i> , 2002, 58, 5141-5145.	1.0	3
122	N-1-alkylitaconamic acids-co-styrene copolymers. Surface characterization. <i>Polymer</i> , 2003, 44, 3969-3975.	1.8	3
123	Antioxidant reactivity toward nitroxide probes anchored into human serum albumin. A new model for studying antioxidant repairing capacity of protein radicals. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009, 19, 6382-6385.	1.0	3
124	Odd Loop Regions of XenA and XenB Enzymes Modulate Their Interaction with Nitro-explosives Compounds and Provide Structural Support for Their Regioselectivity. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3860-3870.	2.5	3
125	Unnexins: Homologs of innexin proteins in <i>Trypanosomatidae</i> parasites. <i>Journal of Cellular Physiology</i> , 2022, 237, 1547-1560.	2.0	3
126	Interaction Energy in Polymer Blends Containing N-1-Alkylitaconamic Acids Moiety. <i>Journal of Macromolecular Science - Physics</i> , 2003, 42, 1281-1291.	0.4	2



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127	Relative solvation and strength of polycyano- and polynitromethanes in water: a study with molecular dynamics simulations. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 128-133.	0.9	2
128	Loss of TP53-DNA interaction induced by p.C135R in lung cancer. <i>Oncology Reports</i> , 2007, , .	1.2	2
129	Novel Insights for Inhibiting Mutant Heterodimer IDH1wt-R132H in Cancer: An In-Silico Approach. <i>Molecular Diagnosis and Therapy</i> , 2018, 22, 369-380.	1.6	2
130	A rationally designed orthogonal synthetase for genetically encoded fluorescent amino acids. <i>Heliyon</i> , 2020, 6, e05140.	1.4	2
131	PLIDflow: an open-source workflow for the online analysis of protein-ligand docking using galaxy. <i>Bioinformatics</i> , 2020, 36, 4203-4205.	1.8	2
132	Loss of TP53-DNA interaction induced by p.C135R in lung cancer. <i>Oncology Reports</i> , 2007, 18, 1213-7.	1.2	2
133	The Emergence of New Catalytic Abilities in an Endoxylanase from Family GH10 by Removing an Intrinsically Disordered Region. <i>International Journal of Molecular Sciences</i> , 2022, 23, 2315.	1.8	2
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