Lennane Michel Espinoza-Fonseca

List of Publications by Year
in descending order

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62 papers	1,435 citations	304743 22 h-index	377865 34 g-index
64 all docs	64 docs citations	64 times ranked	1809 citing authors

#	Article	IF	Citations
1	The benefits of the multi-target approach in drug design and discovery. Bioorganic and Medicinal Chemistry, 2006, 14, 896-897.	3.0	130
2	Reconciling binding mechanisms of intrinsically disordered proteins. Biochemical and Biophysical Research Communications, 2009, 382, 479-482.	2.1	83
3	Phosphorylation-induced structural changes in smooth muscle myosin regulatory light chain. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 8207-8212.	7.1	74
4	Molecular Dynamics Simulations Reveal a Disorder-to-Order Transition on Phosphorylation of Smooth Muscle Myosin. Biophysical Journal, 2007, 93, 2083-2090.	0.5	64
5	Thermodynamic and Structural Basis of Phosphorylation-Induced Disorder-to-Order Transition in the Regulatory Light Chain of Smooth Muscle Myosin. Journal of the American Chemical Society, 2008, 130, 12208-12209.	13.7	57
6	Atomic-Level Characterization of the Activation Mechanism of SERCA by Calcium. PLoS ONE, 2011, 6, e26936.	2.5	50
7	Site-directed spectroscopy of cardiac myosin-binding protein C reveals effects of phosphorylation on protein structural dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 3233-3238.	7.1	47
8	Docking and quantum mechanic studies on cholinesterases and their inhibitors. European Journal of Medicinal Chemistry, 2007, 42, 10-19.	5.5	46
9	Synthesis, anticholinesterase activity and structureâ€“Activity relationships of m-Aminobenzoic acid derivatives. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 1825-1827.	2.2	42
10	Microsecond Molecular Dynamics Simulations of Mg2+- and K+- Bound E1 Intermediate States of the Calcium Pump. PLoS ONE, 2014, 9, e95979.	2.5	39
11	Sarcolipin Promotes Uncoupling of the SERCA Ca²⁺ Pump by Inducing a Structural Rearrangement in the Energy-Transduction Domain. Biochemistry, 2016, 55, 6083-6086.	2.5	39
12	Linking Biochemical and Structural States of SERCA: Achievements, Challenges, and New Opportunities. International Journal of Molecular Sciences, 2020, 21, 4146.	4.1	36
13	pâ€“Aminobenzoic acid derivatives as acetylcholinesterase inhibitors. European Journal of Medicinal Chemistry, 2005, 40, 732-735.	5.5	35
14	Atomic-Level Mechanisms for Phospholamban Regulation of the Calcium Pump. Biophysical Journal, 2015, 108, 1697-1708.	0.5	35
15	Nothing Regular about the Regulins: Distinct Functional Properties of SERCA Transmembrane Peptide Regulatory Subunits. International Journal of Molecular Sciences, 2021, 22, 8891.	4.1	32
16	Leucineâ€rich hydrophobic clusters promote folding of the Nâ€terminus of the intrinsically disordered transactivation domain of p53. FEBS Letters, 2009, 583, 556-560.	2.8	31
17	Aromatic residues link binding and function of intrinsically disordered proteins. Molecular BioSystems, 2012, 8, 237-246.	2.9	31
18	Sarcolipin and phospholamban inhibit the calcium pump by populating a similar metal ion-free intermediate state. Biochemical and Biophysical Research Communications, 2015, 463, 37-41.	2.1	31

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19	Dwarf open reading frame (DWORF) is a direct activator of the sarcoplasmic reticulum calcium pump SERCA. ELife, 2021, 10, .	6.0	31
20	The Phospholamban Pentamer Alters Function of the Sarcoplasmic Reticulum Calcium Pump SERCA. Biophysical Journal, 2019, 116, 633-647.	0.5	30
21	Targeting MDM2 by the small molecule RITA: towards the development of new multi-target drugs against cancer. , 2005, 2, 38.		25
22	Backbone conformational preferences of an intrinsically disordered protein in solution. Molecular BioSystems, 2012, 8, 1798.	2.9	24
23	Aromaticâ€“aromatic interactions in the formation of the MDM2â€“p53 complex. Biochemical and Biophysical Research Communications, 2008, 370, 547-551.	2.1	23
24	Structural considerations for the rational design of selective anti-trypanosomal agents: The role of the aromatic clusters at the interface of triosephosphate isomerase dimer. Biochemical and Biophysical Research Communications, 2005, 328, 922-928.	2.1	22
25	Exploring the possible binding sites at the interface of triosephosphate isomerase dimer as a potential target for anti-tripanosomal drug design. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 3151-3154.	2.2	20
26	The existence of a second allosteric site on the M1 muscarinic acetylcholine receptor and its implications for drug design. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 1217-1220.	2.2	20
27	Structural basis for relief of phospholamban-mediated inhibition of the sarcoplasmic reticulum Ca2+-ATPase at saturating Ca2+ conditions. Journal of Biological Chemistry, 2018, 293, 12405-12414.	3.4	20
28	Toward a rational design of selective multi-trypanosomatid inhibitors: A computational docking study. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 6288-6292.	2.2	19
29	Thermodynamic Aspects of Coupled Binding and Folding of an Intrinsically Disordered Protein: A Computational Alanine Scanning Study. Biochemistry, 2009, 48, 11332-11334.	2.5	19
30	Microsecond Molecular Simulations Reveal a Transient Proton Pathway in the Calcium Pump. Journal of the American Chemical Society, 2015, 137, 7055-7058.	13.7	18
31	Base docking model of the homomeric Î±7 nicotinic receptorâ€“Î²-amyloid1â€“42 complex. Biochemical and Biophysical Research Communications, 2004, 320, 587-591.	2.1	16
32	Transient stability of the helical pattern of region F19â€“L22 of the N-terminal domain of p53: A molecular dynamics simulation study. Biochemical and Biophysical Research Communications, 2006, 343, 110-116.	2.1	15
33	Inhibition of acetylcholinesterase by two arylderivatives: 3a-Acetoxy-5H-pyrrolo(1,2-a) (3,1)benzoxazin-1,5-(3aH)-dione andcis-N-p-Acetoxy-phenylisomaleimide. Journal of Enzyme Inhibition and Medicinal Chemistry, 2006, 21, 133-138.	5.2	15
34	Effects of pseudophosphorylation mutants on the structural dynamics of smooth muscle myosin regulatory light chain. Molecular BioSystems, 2014, 10, 2693-2698.	2.9	15
35	Sequential myosin phosphorylation activates tarantula thick filament via a disorderâ€“order transition. Molecular BioSystems, 2015, 11, 2167-2179.	2.9	15
36	Interaction of a Sarcolipin Pentamer and Monomer with the Sarcoplasmic Reticulum Calcium Pump, SERCA. Biophysical Journal, 2020, 118, 518-531.	0.5	13

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37	Fluorescence lifetime imaging microscopy reveals sodium pump dimers in live cells. Journal of Biological Chemistry, 2022, 298, 101865.	3.4	12
38	Identification of multiple allosteric sites on the M1muscarinic acetylcholine receptor. FEBS Letters, 2005, 579, 6726-6732.	2.8	11
39	Structural Mechanism for Regulation of Bcl-2 protein Noxa by phosphorylation. Scientific Reports, 2015, 5, 14557.	3.3	11
40	Preexisting domain motions underlie protonation-dependent structural transitions of the P-type Ca2+-ATPase. Physical Chemistry Chemical Physics, 2017, 19, 10153-10162.	2.8	11
41	Multiscale Simulation Reveals Passive Proton Transport Through SERCA on the Microsecond Timescale. Biophysical Journal, 2020, 119, 1033-1040.	0.5	11
42	Molecular docking of four Î²-amyloid1â€“42 fragments on the Î±7 nicotinic receptor: delineating the binding site of the AÎ² peptides. Biochemical and Biophysical Research Communications, 2004, 323, 1191-1196.	2.1	10
43	Structure and dynamics of the full-length M1 muscarinic acetylcholine receptor studied by molecular dynamics simulations. Archives of Biochemistry and Biophysics, 2008, 469, 142-150.	3.0	10
44	The Ca²⁺-ATPase pump facilitates bidirectional proton transport across the sarco/endoplasmic reticulum. Molecular BioSystems, 2017, 13, 633-637.	2.9	10
45	A multiscale approach for bridging the gap between potency, efficacy, and safety of small molecules directed at membrane proteins. Scientific Reports, 2021, 11, 16580.	3.3	10
46	Dynamics-Driven Allostery Underlies Ca2+-Mediated Release of SERCA Inhibition by Phospholamban. Biophysical Journal, 2020, 119, 1917-1926.	0.5	10
47	Atomistic Characterization of the First Step of Calcium Pump Activation Associated with Proton Countertransport. Biochemistry, 2015, 54, 5235-5241.	2.5	9
48	Tyr74 is essential for the formation, stability and function of Plasmodium falciparum triosephosphate isomerase dimer. Archives of Biochemistry and Biophysics, 2010, 494, 46-57.	3.0	8
49	Fully flexible docking models of the complex between Î±7 nicotinic receptor and a potent heptapeptide inhibitor of the Î²-amyloid peptide binding. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 3519-3523.	2.2	7
50	Pathogenic mutation R959W alters recognition dynamics of dysferlin inner DysF domain. Molecular BioSystems, 2016, 12, 973-981.	2.9	6
51	Atomistic Structure and Dynamics of the Ca2+-ATPase Bound to Phosphorylated Phospholamban. International Journal of Molecular Sciences, 2020, 21, 7261.	4.1	6
52	Structural Basis for the Limited Response to Oxidative and Thiol-Conjugating Agents by Triosephosphate Isomerase From the Photosynthetic Bacteria Synechocystis. Frontiers in Molecular Biosciences, 2018, 5, 103.	3.5	5
53	Knowledgebase for addiction-related genes: Is it possible an extrapolation to rational multi-target drug design?. Bioorganic and Medicinal Chemistry, 2008, 16, 9346-9348.	3.0	4
54	Dynamic optimization of signal transductionvia intrinsic disorder. Molecular BioSystems, 2012, 8, 194-197.	2.9	4

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55	Probing the effects of nonannular lipid binding on the stability of the calcium pump SERCA. Scientific Reports, 2019, 9, 3349.	3.3	4
56	Homologous cardiac calcium pump regulators phospholamban and sarcolipin adopt distinct oligomeric states in the membrane. Computational and Structural Biotechnology Journal, 2022, 20, 380-384.	4.1	4
57	Conserved Luminal C-Terminal Domain Dynamically Controls Interdomain Communication in Sarcolipin. Journal of Chemical Information and Modeling, 2020, 60, 3985-3991.	5.4	3
58	A hallmark of phospholamban functional divergence is located in the N-terminal phosphorylation domain. Computational and Structural Biotechnology Journal, 2020, 18, 705-713.	4.1	3
59	Primitive Phospholamban- and Sarcolipin-like Peptides Inhibit the Sarcoplasmic Reticulum Calcium Pump SERCA. Biochemistry, 2022, 61, 1419-1430.	2.5	2
60	An in silico pipeline for the discovery of multitarget ligands: A case study for epi-polypharmacology based on DNMT1/HDAC2 inhibition. Artificial Intelligence in the Life Sciences, 2021, 1, 100008.	2.2	1
61	Synthesis, Anticholinesterase Activity and Structureâ€"Activity Relationships of m-Aminobenzoic Acid Derivatives.. ChemInform, 2003, 34, no.	0.0	0
62	Structural Basis for the Function of the C-Terminal Proton Release Pathway in the Calcium Pump. International Journal of Molecular Sciences, 2021, 22, 3507.	4.1	0