Leandro Martinez

List of Publications by Year
in descending order

71 papers	8,137 citations	377584 21 h-index	116156 66 g-index
77 all docs	77 docs citations	77 times ranked	10476 citing authors

#	Article	IF	Citations
1	ComplexMixtures.jl: Investigating the structure of solutions of complex-shaped molecules from a solvent-shell perspective. Journal of Molecular Liquids, 2022, 347, 117945.	2.3	16
2	CellListMap.jl: Efficient and customizable cell list implementation for calculation of pairwise particle properties within a cutoff. Computer Physics Communications, 2022, 279, 108452.	3.0	0
3	Structural discrimination analysis for constraint selection in protein modeling. Bioinformatics, 2021, 37, 3766-3773.	1.8	0
4	Wrapping Up Viruses at Multiscale Resolution: Optimizing PACKMOL and SIRAH Execution for Simulating the Zika Virus. Journal of Chemical Information and Modeling, 2021, 61, 408-422.	2.5	18
5	On the Interpretation of subtilisin Carlsberg Time-Resolved Fluorescence Anisotropy Decays: Modeling with Classical Simulations. Journal of Chemical Information and Modeling, 2020, 60, 747-755.	2.5	3
6	Structural complementarity of distance constraints obtained from chemical crossâ€linking and amino acid coevolution. Proteins: Structure, Function and Bioinformatics, 2020, 88, 625-632.	1.5	2
7	Correlated counterion effects on the solvation of proteins by ionic liquids. Journal of Molecular Liquids, 2020, 320, 114347.	2.3	10
8	Elucidating the Structural Basis of the Intracellular pH Sensing Mechanism of TASK-2 K2P Channels. International Journal of Molecular Sciences, 2020, 21, 532.	1.8	4
9	The shift in urea orientation at protein surfaces at low pH is compatible with a direct mechanism of protein denaturation. Physical Chemistry Chemical Physics, 2020, 22, 354-367.	1.3	19
10	TopoLink: evaluation of structural models using chemical crosslinking distance constraints. Bioinformatics, 2019, 35, 3169-3170.	1.8	16
11	Oncogenic basic amino acid insertions at the extracellular juxtamembrane region of IL7RA cause receptor hypersensitivity. Blood, 2019, 133, 1259-1263.	0.6	6
12	Molecular simulations of fluconazole-mediated inhibition of sterol biosynthesis. Journal of Biomolecular Structure and Dynamics, 2019, 38, 1-11.	2.0	3
13	Statistical force-field for structural modeling using chemical cross-linking/mass spectrometry distance constraints. Bioinformatics, 2019, 35, 3005-3012.	1.8	13
14	Coevolutionary Signals and Structure-Based Models for the Prediction of Protein Native Conformations. Methods in Molecular Biology, 2019, 1851, 83-103.	0.4	9
15	Parametric models to compute tryptophan fluorescence wavelengths from classical protein simulations. Journal of Computational Chemistry, 2018, 39, 1249-1258.	1.5	8
16	Enhancing protein fold determination by exploring the complementary information of chemical cross-linking and coevolutionary signals. Bioinformatics, 2018, 34, 2201-2208.	1.8	13
17	MEASURING THE CONDUCTIVITY OF VERY DILUTE ELECTROLYTE SOLUTIONS, DROP BY DROP. Quimica Nova, 2018, , .	0.3	2
18	Prediction of kinetics of protein folding with non-redundant contact information. Bioinformatics, 2018, 34, 4034-4038.	1.8	9

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19	A network model predicts the intensity of residue-protein thermal coupling. Bioinformatics, 2017, 33, 2106-2113.	1.8	7
20	Molecular Interpretation of Preferential Interactions in Protein Solvation: A Solvent-Shell Perspective by Means of Minimum-Distance Distribution Functions. Journal of Chemical Theory and Computation, 2017, 13, 6358-6372.	2.3	39
21	Molecular mechanism of activation of Burkholderia cepacia lipase at aqueousâ€“organic interfaces. Physical Chemistry Chemical Physics, 2017, 19, 31499-31507.	1.3	14
22	Molecular basis for competitive solvation of the Burkholderia cepacia lipase by sorbitol and urea. Physical Chemistry Chemical Physics, 2016, 18, 21797-21808.	1.3	14
23	Anthrax Edema Factor: An Ion-Adaptive Mechanism of Catalysis with Increased Transition-State Conformational Flexibility. Journal of Physical Chemistry B, 2016, 120, 6504-6514.	1.2	7
24	Conformational Diversity of the Helix 12 of the Ligand Binding Domain of PPARÎ³ and Functional Implications. Journal of Physical Chemistry B, 2015, 119, 15418-15429.	1.2	14
25	Automatic Identification of Mobile and Rigid Substructures in Molecular Dynamics Simulations and Fractional Structural Fluctuation Analysis. PLoS ONE, 2015, 10, e0119264.	1.1	320
26	Identification of a New Hormone-Binding Site on the Surface of Thyroid Hormone Receptor. Molecular Endocrinology, 2014, 28, 534-545.	3.7	33
27	Introducing the Levinthalâ€™s Protein Folding Paradox and Its Solution. Journal of Chemical Education, 2014, 91, 1918-1923.	1.1	15
28	Small-angle X-ray scattering and structural modeling of full-length: cellobiohydrolase I from Trichoderma harzianum. Cellulose, 2013, 20, 1573-1585.	2.4	10
29	Dynamics of Nuclear Receptor Helix-12 Switch of Transcription Activation by Modeling Time-Resolved Fluorescence Anisotropy Decays. Biophysical Journal, 2013, 105, 1670-1680.	0.2	34
30	Sparse Projected-Gradient Method As a Linear-Scaling Low-Memory Alternative to Diagonalization in Self-Consistent Field Electronic Structure Calculations. Journal of Chemical Theory and Computation, 2013, 9, 1043-1051.	2.3	11
31	Molecular Motions as a Drug Target: Mechanistic Simulations of Anthrax Toxin Edema Factor Function Led to the Discovery of Novel Allosteric Inhibitors. Toxins, 2012, 4, 580-604.	1.5	18
32	Enzyme Microheterogeneous Hydration and Stabilization in Supercritical Carbon Dioxide. Journal of Physical Chemistry B, 2012, 116, 5671-5678.	1.2	37
33	Hb S-SÃ£o Paulo: A new sickling hemoglobin with stable polymers and decreased oxygen affinity. Archives of Biochemistry and Biophysics, 2012, 519, 23-31.	1.4	10
34	Medium Chain Fatty Acids Are Selective Peroxisome Proliferator Activated Receptor (PPAR) Î³ Activators and Pan-PPAR Partial Agonists. PLoS ONE, 2012, 7, e36297.	1.1	165
35	Molecular Basis of the Thermostability and Thermophilicity of Laminarinases: X-ray Structure of the Hyperthermostable Laminarinase from Rhodothermus marinus and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 7940-7949.	1.2	26
36	Mapping the Intramolecular Vibrational Energy Flow in Proteins Reveals Functionally Important Residues. Journal of Physical Chemistry Letters, 2011, 2, 2073-2078.	2.1	41

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37	Helix 12 Dynamics and Thyroid Hormone Receptor Activity: Experimental and Molecular Dynamics Studies of Ile280 Mutants. Journal of Molecular Biology, 2011, 412, 882-893.	2.0	15
38	Inexact restoration method for minimization problems arising in electronic structure calculations. Computational Optimization and Applications, 2011, 50, 555-590.	0.9	14
39	Molecular characterization of a miraculin-like gene differentially expressed during coffee development and coffee leaf miner infestation. Planta, 2011, 233, 123-137.	1.6	22
40	The redundancy of NMR restraints can be used to accelerate the unfolding behavior of an SH3 domain during molecular dynamics simulations. BMC Structural Biology, 2011, 11, 46.	2.3	1
41	Mechanism of reactant and product dissociation from the anthrax edema factor: A locally enhanced sampling and steered molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1649-1661.	1.5	7
42	CHARMM force field parameterization of rosiglitazone. International Journal of Quantum Chemistry, 2011, 111, 1346-1354.	1.0	13
43	Analysis of Agonist and Antagonist Effects on Thyroid Hormone Receptor Conformation by Hydrogen/Deuterium Exchange. Molecular Endocrinology, 2011, 25, 15-31.	3.7	41
44	Structural modeling of high-affinity thyroid receptorâ€“ligand complexes. European Biophysics Journal, 2010, 39, 1523-1536.	1.2	12
45	Activation of the Edema Factor of Bacillus anthracis by Calmodulin: Evidence of an Interplay between the EF-Calmodulin Interaction andÂCalcium Binding. Biophysical Journal, 2010, 99, 2264-2272.	0.2	16
46	On the Denaturation Mechanisms of the Ligand Binding Domain of Thyroid Hormone Receptors. Journal of Physical Chemistry B, 2010, 114, 1529-1540.	1.2	8
47	Gaining ligand selectivity in thyroid hormone receptors via entropy. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 20717-20722.	3.3	76
48	P<scp>ACKMOL</scp>: A package for building initial configurations for molecular dynamics simulations. Journal of Computational Chemistry, 2009, 30, 2157-2164.	1.5	5,831
49	Low Order-Value Optimization and applications. Journal of Global Optimization, 2009, 43, 1-22.	1.1	16
50	ATP conformations and ion binding modes in the active site of anthrax edema factor: A computational analysis. Proteins: Structure, Function and Bioinformatics, 2009, 77, 971-983.	1.5	13
51	Structural basis of GC-1 selectivity for thyroid hormone receptor isoforms. BMC Structural Biology, 2008, 8, 8.	2.3	42
52	Only Subtle Protein Conformational Adaptations Are Required for Ligand Binding to Thyroid Hormone Receptors: Simulations Using a Novel Multipoint Steered Molecular Dynamics Approach. Journal of Physical Chemistry B, 2008, 112, 10741-10751.	1.2	51
53	Ligand Dissociation from Estrogen Receptor Is Mediated by Receptor Dimerization: Evidence from Molecular Dynamics Simulations. Molecular Endocrinology, 2008, 22, 1565-1578.	3.7	54
54	Trust-region superposition methods for protein alignment. IMA Journal of Numerical Analysis, 2008, 28, 690-710.	1.5	4

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55	Convergent algorithms for protein structural alignment. BMC Bioinformatics, 2007, 8, 306.	1.2	72
56	Continuous optimization methods for structure alignments. Mathematical Programming, 2007, 112, 93-124.	1.6	13
57	Molecular Dynamics Simulations of Ligand Dissociation from Thyroid Hormone Receptors:Â Evidence of the Likeliest Escape Pathway and Its Implications for the Design of Novel Ligands. Journal of Medicinal Chemistry, 2006, 49, 23-26.	2.9	73
58	Density-based Globally Convergent Trust-region Methods for Self-consistent Field Electronic Structure Calculations. Journal of Mathematical Chemistry, 2006, 40, 349-377.	0.7	20
59	Molecular Dynamics Simulations Reveal Multiple Pathways of Ligand Dissociation from Thyroid Hormone Receptors. Biophysical Journal, 2005, 89, 2011-2023.	0.2	66
60	A review on the dynamics of water. Brazilian Journal of Physics, 2004, 34, 3-16.	0.7	22
61	Globally convergent trust-region methods for self-consistent field electronic structure calculations. Journal of Chemical Physics, 2004, 121, 10863.	1.2	36
62	Packing optimization for automated generation of complex system's initial configurations for molecular dynamics and docking. Journal of Computational Chemistry, 2003, 24, 819-825.	1.5	556
63	Synthesis, characterization and catalytic properties of solâ€“gel derived mixed oxides. Journal of Physics and Chemistry of Solids, 2003, 64, 2385-2389.	1.9	32
64	Thermochemical data on adducts of copper chloride with the amino acids lysine and glycine. Thermochimica Acta, 2002, 395, 21-26.	1.2	7
65	A calorimetric investigation into copperâ€“arginine and copperâ€“alanine solid state interactions. Transition Metal Chemistry, 2002, 27, 253-255.	0.7	9
66	Title is missing!. Transition Metal Chemistry, 2002, 27, 748-750.	0.7	8
67	Synthesis, characterization and thermal behavior of 18 cadmium halides adducts involving ethyleneurea, ethylenethiourea and propyleneurea. Thermochimica Acta, 2001, 376, 91-94.	1.2	12
68	Decrease of interlamellar spacing of silica samples induced by external pressure. Journal of Non-Crystalline Solids, 2000, 276, 56-60.	1.5	8
69	Structural Complementarity of Distance Constraints Obtained from Chemical Crosslinking and Amino Acid Coevolution. SSRN Electronic Journal, 0, , .	0.4	0
70	Conceitos bÃ¡sicos de computaÃ§Ã£o cientÃfica: fundamentos da simulaÃ§Ã£o de sistemas fÃsicos. , 0, , .		0
71	AnÃ¡lise do Comportamento de AplicaÃ§Ãµes Paralelas em Ambientes de ComputaÃ§Ã£o de Alto Desempenho Virtualizados. , 0, , .		0