Diogo Vila-ViÃ§osa

List of Publications by Year
in descending order

36 papers	929 citations	361045 20 h-index	476904 29 g-index
36 all docs	36 docs citations	36 times ranked	1273 citing authors

#	Article	IF	Citations
1	pK_a Values of Titrable Amino Acids at the Water/Membrane Interface. Journal of Chemical Theory and Computation, 2016, 12, 930-934.	2.3	59
2	Targeting Type 2 Diabetes withC-Glucosyl Dihydrochalcones as Selective Sodium Glucose Co-Transporter 2 (SGLT2) Inhibitors: Synthesis and Biological Evaluation. Journal of Medicinal Chemistry, 2017, 60, 568-579.	2.9	50
3	Luminescent Diâ€•and Trinuclear Boron Complexes Based on Aromatic Iminopyrrolyl Spacer Ligands: Synthesis, Characterization, and Application in OLEDs. Chemistry - A European Journal, 2015, 21, 9133-9149.	1.7	47
4	Differential targeting of membrane lipid domains by caffeic acid and its ester derivatives. Free Radical Biology and Medicine, 2018, 115, 232-245.	1.3	42
5	Reversibility of Prion Misfolding: Insights from Constant-pH Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 8812-8821.	1.2	41
6	Constant-pH MD Simulations of DMPA/DMPC Lipid Bilayers. Journal of Chemical Theory and Computation, 2015, 11, 5973-5979.	2.3	36
7	Boron complexes of aromatic ring fused iminopyrrolyl ligands: synthesis, structure, and luminescence properties. Dalton Transactions, 2016, 45, 15603-15620.	1.6	36
8	Halogen bonding in halocarbon-protein complexes and computational tools for rational drug design. Expert Opinion on Drug Discovery, 2019, 14, 805-820.	2.5	36
9	Coordination-driven self-assembly of thiocyanate complexes of Co(ii), Ni(ii) and Cu(ii) with picolinamide: a structural and DFT study. CrystEngComm, 2011, 13, 5863.	1.3	35
10	A Simulated Intermediate State for Folding and Aggregation Provides Insights into Î”N6 Î²2-Microglobulin Amyloidogenic Behavior. PLoS Computational Biology, 2014, 10, e1003606.	1.5	34
11	Halogen Bonding: An Underestimated Player in Membraneâ€“Ligand Interactions. Journal of the American Chemical Society, 2021, 143, 4253-4267.	6.6	34
12	Dinuclear Zincâ€“Nâ€•Heterocyclic Carbene Complexes for Either the Controlled Ringâ€•Opening Polymerization of Lactide or the Controlled Degradation of Polylactide Under Mild Conditions. ChemCatChem, 2014, 6, 1357-1367.	1.8	33
13	The Impact of Using Single Atomistic Long-Range Cutoff Schemes with the GROMOS 54A7 Force Field. Journal of Chemical Theory and Computation, 2018, 14, 5823-5833.	2.3	33
14	Membrane-Induced pK_a Shifts in wt-pHLIP and Its L16H Variant. Journal of Chemical Theory and Computation, 2018, 14, 3289-3297.	2.3	33
15	PypKa: A Flexible Python Module for Poissonâ€“Boltzmann-Based pK_a Calculations. Journal of Chemical Information and Modeling, 2020, 60, 4442-4448.	2.5	33
16	Sugar-based bactericides targeting phosphatidylethanolamine-enriched membranes. Nature Communications, 2018, 9, 4857.	5.8	31
17	Constant-pH MD Simulations of an Oleic Acid Bilayer. Journal of Chemical Theory and Computation, 2015, 11, 2367-2376.	2.3	30
18	Conformational Study of GSH and GSSG Using Constant-pH Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 7507-7517.	1.2	29

#	Article	IF	Citations
19	Protonation of DMPC in a Bilayer Environment Using a Linear Response Approximation. Journal of Chemical Theory and Computation, 2014, 10, 2176-2184.	2.3	29
20	Treatment of Ionic Strength in Biomolecular Simulations of Charged Lipid Bilayers. Journal of Chemical Theory and Computation, 2014, 10, 5483-5492.	2.3	23
21	Role of Counterions in Constant-pH Molecular Dynamics Simulations of PAMAM Dendrimers. ACS Omega, 2018, 3, 2001-2009.	1.6	20
22	Biomolecular Simulations of Halogen Bonds with a GROMOS Force Field. Journal of Chemical Theory and Computation, 2018, 14, 5383-5392.	2.3	20
23	Wittig Reaction: Domino Olefination and Stereoselectivity DFT Study. Synthesis of the Miharamycinsâ€™ Bicyclic Sugar Moiety. Organic Letters, 2015, 17, 5622-5625.	2.4	18
24	A tale of two tails: The importance of unstructured termini in the aggregation pathway of Î²2â€microglobulin. Proteins: Structure, Function and Bioinformatics, 2017, 85, 2045-2057.	1.5	17
25	Violet-blue emitting 2-(N-alkylimino)pyrrolyl organoboranes: Synthesis, structure and luminescent properties. Dyes and Pigments, 2017, 140, 520-532.	2.0	17
26	A pH Replica Exchange Scheme in the Stochastic Titration Constant-pH MD Method. Journal of Chemical Theory and Computation, 2019, 15, 3108-3116.	2.3	17
27	Insights on the Mechanism of Action of INH-C₁₀ as an Antitubercular Prodrug. Molecular Pharmaceutics, 2017, 14, 4597-4605.	2.3	15
28	Tackling Halogenated Species with PBSA: Effect of Emulating the Ïƒ-Hole. Journal of Chemical Theory and Computation, 2019, 15, 4241-4251.	2.3	15
29	New luminescent tetracoordinate boron complexes: an in-depth experimental and theoretical characterisation and their application in OLEDs. Inorganic Chemistry Frontiers, 2021, 8, 3960-3983.	3.0	13
30	Improved Protocol to Tackle the pH Effects on Membrane-Inserting Peptides. Journal of Chemical Theory and Computation, 2021, 17, 3830-3840.	2.3	12
31	The Early Phase of Î²2m Aggregation: An Integrative Computational Study Framed on the D76N Mutant and the Î”N6 Variant. Biomolecules, 2019, 9, 366.	1.8	11
32	Can self-assembly of copper(ii) picolinamide building blocks be controlled?. CrystEngComm, 2013, 15, 8074.	1.3	9
33	Why a diaminopyrrolic tripodal receptor binds mannosides in acetonitrile but not in water?. Beilstein Journal of Organic Chemistry, 2014, 10, 1513-1523.	1.3	6
34	Identification of Pan-Assay INterference compoundS (PAINS) Using an MD-Based Protocol. Methods in Molecular Biology, 2021, 2315, 263-271.	0.4	6
35	Optimization of an in Silico Protocol Using Probe Permeabilities to Identify Membrane Pan-Assay Interference Compounds. Journal of Chemical Information and Modeling, 2022, 62, 3034-3042.	2.5	5
36	Unsupervised Walking Activity Assessment Reveals <scp>COVID</scp>â€19 Impact on Parkinson's Disease Patients. Movement Disorders, 2021, 36, 531-532.	2.2	4