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	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
2	Identification of Pan-Assay INterference compoundS (PAINS) Using an MD-Based Protocol. Methods in Molecular Biology, 2021, 2315, 263-271.	0.4	6
3	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
4	Halogen Bonding: An Underestimated Player in Membraneâ€“Ligand Interactions. Journal of the American Chemical Society, 2021, 143, 4253-4267.	6.6	34
5	Improved Protocol to Tackle the pH Effects on Membrane-Inserting Peptides. Journal of Chemical Theory and Computation, 2021, 17, 3830-3840.	2.3	12
6	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
7	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
8	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
9	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
10	Tackling Halogenated Species with PBSA: Effect of Emulating the Ï*f*-Hole. Journal of Chemical Theory and Computation, 2019, 15, 4241-4251.	2.3	15
11	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
12	Role of Counterions in Constant-pH Molecular Dynamics Simulations of PAMAM Dendrimers. ACS Omega, 2018, 3, 2001-2009.	1.6	20
13	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
14	Sugar-based bactericides targeting phosphatidylethanolamine-enriched membranes. Nature Communications, 2018, 9, 4857.	5.8	31
15	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
16	Biomolecular Simulations of Halogen Bonds with a GROMOS Force Field. Journal of Chemical Theory and Computation, 2018, 14, 5383-5392.	2.3	20
17	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
18	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

#	Article	IF	Citations
19	Insights on the Mechanism of Action of INH-C₁₀ as an Antitubercular Prodrug. Molecular Pharmaceutics, 2017, 14, 4597-4605.	2.3	15
20	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
21	Violet-blue emitting 2-(N-alkylimino)pyrrolyl organoboranes: Synthesis, structure and luminescent properties. Dyes and Pigments, 2017, 140, 520-532.	2.0	17
22	Boron complexes of aromatic ring fused iminopyrrolyl ligands: synthesis, structure, and luminescence properties. Dalton Transactions, 2016, 45, 15603-15620.	1.6	36
23	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
24	Constant-pH MD Simulations of an Oleic Acid Bilayer. Journal of Chemical Theory and Computation, 2015, 11, 2367-2376.	2.3	30
25	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
26	Constant-pH MD Simulations of DMPA/DMPC Lipid Bilayers. Journal of Chemical Theory and Computation, 2015, 11, 5973-5979.	2.3	36
27	Wittig Reaction: Domino Olefination and Stereoselectivity DFT Study. Synthesis of the Miharamycinsâ€™ Bicyclic Sugar Moiety. Organic Letters, 2015, 17, 5622-5625.	2.4	18
28	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
29	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
30	Treatment of Ionic Strength in Biomolecular Simulations of Charged Lipid Bilayers. Journal of Chemical Theory and Computation, 2014, 10, 5483-5492.	2.3	23
31	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
32	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
33	Can self-assembly of copper(ii) picolinamide building blocks be controlled?. CrystEngComm, 2013, 15, 8074.	1.3	9
34	Conformational Study of GSH and GSSG Using Constant-pH Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 7507-7517.	1.2	29
35	Reversibility of Prion Misfolding: Insights from Constant-pH Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 8812-8821.	1.2	41
36	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