Luis G. Dias

List of Publications by Year in descending order

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LUIS C. DIAS

#	Article	lF	CITATIONS
1	Modulation of methylene blue photochemical properties based on adsorption at aqueous micelle interfaces. Physical Chemistry Chemical Physics, 2002, 4, 2320-2328.	2.8	222
2	Parallel damage in mitochondria and lysosomes is an efficient way to photoinduce cell death. Autophagy, 2019, 15, 259-279.	9.1	111
3	A Mixed Culture of Endophytic Fungi Increases Production of Antifungal Polyketides. Journal of Chemical Ecology, 2013, 39, 1335-1342.	1.8	68
4	Effect of Urea on Biomimetic Systems:Â Neither Water 3-D Structure Rupture nor Direct Mechanism, Simply a More "Polar Water― Langmuir, 2002, 18, 319-324.	3.5	64
5	Resonance Raman study of polyynes encapsulated in single-wall carbon nanotubes. Physical Review B, 2007, 76, .	3.2	51
6	Developing electrodes chemically modified with cucurbit[6]uril to detect 3,4-methylenedioxymethamphetamine (MDMA) by voltammetry. Electrochimica Acta, 2014, 121, 188-193.	5.2	44
7	An overview of molecular dynamics simulations of oxidized lipid systems, with a comparison of ELBA and MARTINI force fields for coarse grained lipid simulations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2498-2511.	2.6	41
8	Diketopiperazines produced by endophytic fungi found in association with two Asteraceae species. Phytochemistry, 2010, 71, 1423-1429.	2.9	40
9	Development of constant-pH simulation methods in implicit solvent and applications in biomolecular systems. Biophysical Reviews, 2017, 9, 699-728.	3.2	40
10	A computational study of substituted flavylium salts and their quinonoidal conjugate-bases: SO -> S1 electronic transition, absolute pKa and reduction potential calculations by DFT and semiempirical methods. Journal of the Brazilian Chemical Society, 2007, 18, 1537-1546.	0.6	38
11	Electrostatics analysis of the mutational and pH effects of the N-terminal domain self-association of the major ampullate spidroin. Soft Matter, 2016, 12, 5600-5612.	2.7	38
12	Myclobutanil enantioselective risk assessment in humans through in vitro CYP450 reactions: Metabolism and inhibition studies. Food and Chemical Toxicology, 2019, 128, 202-211.	3.6	36
13	Effect of Counterions on the Shape, Hydration, and Degree of Order at the Interface of Cationic Micelles: The Triflate Case. Langmuir, 2013, 29, 4193-4203.	3.5	33
14	Parameterization of the electronegativity equalization method based on the charge model 1. Physical Chemistry Chemical Physics, 2002, 4, 5933-5936.	2.8	31
15	Theoretical Investigation of the Na ⁺ Transport Mechanism and the Performance of Ionic Liquid-Based Electrolytes in Sodium-Ion Batteries. ACS Applied Energy Materials, 2021, 4, 4444-4458.	5.1	27
16	In vitro enantioselective study of the toxicokinetic effects of chiral fungicide tebuconazole in human liver microsomes. Ecotoxicology and Environmental Safety, 2019, 181, 96-105.	6.0	26
17	Analysis of the Bromide Ion Distribution in the Water Pool of Reverse Micelles of Hexadecyltrimethylammonium Bromide in Chloroform/n-Dodecane and Isooctane/n-Hexanol by Chemical Trapping. Langmuir, 2001, 17, 1060-1068.	3.5	23
18	Molecular Dynamics Simulations of Polymer–Ionic Liquid (1-Ethyl-3-methylimidazolium) Tj ETQq0 0 0 rgBT /C	verlock 10	Tf 50 67 Td (1

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19	Critical Micelle Concentration and Average Aggregation Number Estimate of Zwitterionic Amphiphiles:  Salt Effect. Langmuir, 1997, 13, 5756-5758.	3.5	22
20	Hydrolysis of 1,8- and 2,3-naphthalic anhydrides and the mechanism of cyclization of 1,8-naphthalic acid in aqueous solutionsThe IUPAC name for naphthalic acid is napthalenedicarboxylic acid.Electronic supplementary information (ESI) available: tables containing the values of the rate constants. See http://www.rsc.org/suppdata/p2/b1/b104148g/. Perkin Transactions II RSC, 2001, , 2242-2250	1.1	22
21	Calculation of the Dipole Moment for Polypeptides Using the Generalized Born-Electronegativity Equalization Method:  Results in Vacuum and Continuum-Dielectric Solvent. Journal of Physical Chemistry B, 2004, 108, 4171-4177.	2.6	22
22	Labaditin, a cyclic peptide with rich biotechnological potential: preliminary toxicological studies and structural changes in water and lipid membrane environment. Amino Acids, 2011, 40, 135-144.	2.7	22
23	1-(2-Quinolyl)-2-naphthol: A new intra-intermolecular photoacid–photobase molecule. Journal of Photochemistry and Photobiology A: Chemistry, 2008, 194, 37-48.	3.9	19
24	Chemical identification in the (100) surface using scanning tunneling microscopy and first-principles calculations. Surface Science, 2007, 601, 5540-5545.	1.9	16
25	Aggregation of photosensitizers: the role of dispersion and solvation on dimer formation energetics. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	16
26	New perylenequinone derivatives from the endophytic fungus Alternaria tenuissima SS77. Tetrahedron Letters, 2016, 57, 3185-3189.	1.4	15
27	Interactions between 1â€butylâ€3â€methylimidazolium tetrafluoroborate ionic liquid and γâ€Al ₂ O ₃ (100) surface calculated by density functional theory. International Journal of Quantum Chemistry, 2012, 112, 3234-3239.	2.0	14
28	Self-Assembly of Phosphocholine Derivatives Using the ELBA Coarse-Grained Model: Micelles, Bicelles, and Reverse Micelles. Journal of Chemical Information and Modeling, 2020, 60, 522-536.	5.4	13
29	Substituent effects on the pHâ€dependent multiequilibria of flavylium salt analogs of anthocyanins. Journal of Physical Organic Chemistry, 2011, 24, 1201-1208.	1.9	12
30	Synthesis and spectroscopic properties of luminescent tantalum(v)-β-diketonate complexes and their use as optical sensors and the preparation of nanostructured Ta2O5. Dalton Transactions, 2015, 44, 3829-3836.	3.3	11
31	Methylene Blue Location in (Hydroperoxized) Cardiolipin Monolayer: Implication in Membrane Photodegradation. Journal of Physical Chemistry B, 2017, 121, 8512-8522.	2.6	10
32	Predicting Hydration Free Energies of Neutral Compounds by a Parametrization of the Polarizable Continuum Model. Journal of Physical Chemistry A, 2005, 109, 11322-11327.	2.5	9
33	Signatures of oxygen on <mml:math <br="" xmlns:mml="http://www.w3.org/1998/Math/MathML">display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mn>3 From isolated impurity to oxide regimes. Physical Review B, 2010, 82, .</mml:mn></mml:msub></mml:mrow></mml:math>	3< ∌n₂ ml:mr	s>タ/mml:ms
34	Ion dehydration controls adsorption at the micellar interface: hydrotropic ions. Physical Chemistry Chemical Physics, 2017, 19, 30658-30666.	2.8	9
35	Experimental mapping of a pH gradient from a positively charged micellar interface to bulk solution. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, 611, 125770.	4.7	9
36	Tuning aprotic solvent properties with long alkyl chain ionic liquid for lithium-based electrolytes. Journal of Materials Chemistry A, 2022, 10, 11684-11701.	10.3	9

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37	Ab initio studies of pristine and oxidized Cu3Au(100) and (111) surfaces. Journal of Materials Science, 2012, 47, 7594-7600.	3.7	7
38	Self-assembled films from chitosan and poly(vinyl sulfonic acid) on Nafion® for direct methanol fuel cell. Journal of the Brazilian Chemical Society, 2012, 23, 531-537.	0.6	6
39	Interaction of cyclic and linear Labaditin peptides with anionic and zwitterionic micelles. Journal of Colloid and Interface Science, 2015, 438, 39-46.	9.4	6
40	Development of coarse-grained force field to investigate sodium-ion transport mechanisms in cyanoborate-based ionic liquid. Journal of Molecular Liquids, 2021, 338, 116648.	4.9	6
41	Single-beam interface thermal lensing. Applied Optics, 1999, 38, 1213.	2.1	5
42	Molecular Dynamics Simulations of the Initial-State Predict Product Distributions of Dediazoniation of Aryldiazonium in Binary Solvents. Journal of Organic Chemistry, 2015, 80, 8637-8642.	3.2	5
43	Counterion-mediated Ca2+ accumulation on cationic Langmuir-Blodgett films as template for CaCO3 growth. Thin Solid Films, 2017, 638, 433-440.	1.8	5
44	Citronellal assumes a folded conformation in solution due to dispersion interactions: A joint NMR-DFT analysis. Journal of Molecular Structure, 2018, 1157, 401-407.	3.6	5
45	Parameterization of a coarse-grained model of cholesterol with point-dipole electrostatics. Journal of Computer-Aided Molecular Design, 2018, 32, 1259-1271.	2.9	5
46	Synergistic long-range effects of mutations underlie aggregation propensities of amylin analogues. Journal of Molecular Modeling, 2019, 25, 263.	1.8	5
47	In vitro enantioselective inhibition of the main human CYP450 enzymes involved in drug metabolism by the chiral pesticide tebuconazole. Toxicology Letters, 2021, 351, 1-9.	0.8	5
48	A simple method for the fast calculation of charge redistribution of solutes in an implicit solvent model. Chemical Physics, 2002, 282, 237-243.	1.9	4
49	An Explanation about the Use of (S)-Citronellal as a Chiral Derivatizing Agent (CDA) in 1H and 13C NMR for Sec-Butylamine, Methylbenzylamine, and Amphetamine: A Theoretical-Experimental Study. Molecules, 2019, 24, 2830.	3.8	4
50	Computational insights into substituent effects on the stability and reactivity of flavylium cation analogs of anthocyanins. Arkivoc, 2020, 2020, 146-162.	0.5	2
51	Osmotic Method for Calculating Surface Pressure of Monolayers in Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2022, , .	5.3	2
52	SSPBE: um programa para solução numérica da equação de Poisson-Boltzmann em simetria esférica com modelo de adsorção. Quimica Nova, 2002, 25, 1029-1033.	0.3	0
53	Assessment of Solute-Micelle Interactions in Electrokinetic Chromatography Using Quantitative Structure-Retention Relationships. , 0, , 345-366.		0