

Luis G. Dias

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/5339808/publications.pdf>

Version: 2024-02-01

53
papers

1,287
citations

331259

21
h-index

377514

34
g-index

53
all docs

53
docs citations

53
times ranked

2431
citing authors

#	ARTICLE	IF	CITATIONS
1	Modulation of methylene blue photochemical properties based on adsorption at aqueous micelle interfaces. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 2320-2328.	1.3	222
2	Parallel damage in mitochondria and lysosomes is an efficient way to photoinduce cell death. <i>Autophagy</i> , 2019, 15, 259-279.	4.3	111
3	A Mixed Culture of Endophytic Fungi Increases Production of Antifungal Polyketides. <i>Journal of Chemical Ecology</i> , 2013, 39, 1335-1342.	0.9	68
4	Effect of Urea on Biomimetic Systems: Neither Water 3-D Structure Rupture nor Direct Mechanism, Simply a More Polar Water. <i>Langmuir</i> , 2002, 18, 319-324.	1.6	64
5	Resonance Raman study of polyynes encapsulated in single-wall carbon nanotubes. <i>Physical Review B</i> , 2007, 76, .	1.1	51
6	Developing electrodes chemically modified with cucurbit[6]uril to detect 3,4-methylenedioxymethamphetamine (MDMA) by voltammetry. <i>Electrochimica Acta</i> , 2014, 121, 188-193.	2.6	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. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 2498-2511.	1.4	41
8	Diketopiperazines produced by endophytic fungi found in association with two Asteraceae species. <i>Phytochemistry</i> , 2010, 71, 1423-1429.	1.4	40
9	Development of constant-pH simulation methods in implicit solvent and applications in biomolecular systems. <i>Biophysical Reviews</i> , 2017, 9, 699-728.	1.5	40
10	A computational study of substituted flavylum salts and their quinonoidal conjugate-bases: S0 & S1 electronic transition, absolute pKa and reduction potential calculations by DFT and semiempirical methods. <i>Journal of the Brazilian Chemical Society</i> , 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. <i>Soft Matter</i> , 2016, 12, 5600-5612.	1.2	38
12	Myclobutanil enantioselective risk assessment in humans through in vitro CYP450 reactions: Metabolism and inhibition studies. <i>Food and Chemical Toxicology</i> , 2019, 128, 202-211.	1.8	36
13	Effect of Counterions on the Shape, Hydration, and Degree of Order at the Interface of Cationic Micelles: The Triflate Case. <i>Langmuir</i> , 2013, 29, 4193-4203.	1.6	33
14	Parameterization of the electronegativity equalization method based on the charge model 1. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5933-5936.	1.3	31
15	Theoretical Investigation of the Na ⁺ Transport Mechanism and the Performance of Ionic Liquid-Based Electrolytes in Sodium-Ion Batteries. <i>ACS Applied Energy Materials</i> , 2021, 4, 4444-4458.	2.5	27
16	In vitro enantioselective study of the toxicokinetic effects of chiral fungicide tebuconazole in human liver microsomes. <i>Ecotoxicology and Environmental Safety</i> , 2019, 181, 96-105.	2.9	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. <i>Langmuir</i> , 2001, 17, 1060-1068.	1.6	23
18	Molecular Dynamics Simulations of Polymer-Ionic Liquid (1-Ethyl-3-methylimidazolium) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 67 Td (T Information and Modeling, 2020, 60, 485-499.	2.5	23

#	ARTICLE	IF	CITATIONS
19	Critical Micelle Concentration and Average Aggregation Number Estimate of Zwitterionic Amphiphiles: Salt Effect. <i>Langmuir</i> , 1997, 13, 5756-5758.	1.6	22
20	Hydrolysis of 1,8- and 2,3-naphthalic anhydrides and the mechanism of cyclization of 1,8-naphthalic acid in aqueous solutions The IUPAC name for naphthalic acid is naphthalenedicarboxylic acid. Electronic supplementary information (ESI) available: tables containing the values of the rate constants. See http://www.rsc.org/suppdata/p2/b1/b104148g/ . <i>Perkin Transactions II RSC</i> , 2001, , 2342-2350.	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. <i>Journal of Physical Chemistry B</i> , 2004, 108, 4171-4177.	1.2	22
22	Labaditin, a cyclic peptide with rich biotechnological potential: preliminary toxicological studies and structural changes in water and lipid membrane environment. <i>Amino Acids</i> , 2011, 40, 135-144.	1.2	22
23	1-(2-Quinolyl)-2-naphthol: A new intra-intermolecular photoacid–photobase molecule. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2008, 194, 37-48.	2.0	19
24	Chemical identification in the (100) surface using scanning tunneling microscopy and first-principles calculations. <i>Surface Science</i> , 2007, 601, 5540-5545.	0.8	16
25	Aggregation of photosensitizers: the role of dispersion and solvation on dimer formation energetics. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	16
26	New perylenequinone derivatives from the endophytic fungus <i>Alternaria tenuissima</i> SS77. <i>Tetrahedron Letters</i> , 2016, 57, 3185-3189.	0.7	15
27	Interactions between 1-butyl-3-methylimidazolium tetrafluoroborate ionic liquid and Al_2O_3 (100) surface calculated by density functional theory. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3234-3239.	1.0	14
28	Self-Assembly of Phosphocholine Derivatives Using the ELBA Coarse-Grained Model: Micelles, Bicelles, and Reverse Micelles. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 522-536.	2.5	13
29	Substituent effects on the pH-dependent multiequilibria of flavylum salt analogs of anthocyanins. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 1201-1208.	0.9	12
30	Synthesis and spectroscopic properties of luminescent tantalum(V)- η^2 -diketonate complexes and their use as optical sensors and the preparation of nanostructured Ta ₂ O ₅ . <i>Dalton Transactions</i> , 2015, 44, 3829-3836.	1.6	11
31	Methylene Blue Location in (Hydroperoxized) Cardiolipin Monolayer: Implication in Membrane Photodegradation. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8512-8522.	1.2	10
32	Predicting Hydration Free Energies of Neutral Compounds by a Parametrization of the Polarizable Continuum Model. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11322-11327.	1.1	9
33	Signatures of oxygen on Cu_3O From isolated impurity to oxide regimes. <i>Physical Review B</i> , 2010, 82, .		
34	Ion dehydration controls adsorption at the micellar interface: hydrotropic ions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30658-30666.	1.3	9
35	Experimental mapping of a pH gradient from a positively charged micellar interface to bulk solution. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 611, 125770.	2.3	9
36	Tuning aprotic solvent properties with long alkyl chain ionic liquid for lithium-based electrolytes. <i>Journal of Materials Chemistry A</i> , 2022, 10, 11684-11701.	5.2	9

#	ARTICLE	IF	CITATIONS
37	Ab initio studies of pristine and oxidized Cu ₃ Au(100) and (111) surfaces. <i>Journal of Materials Science</i> , 2012, 47, 7594-7600.	1.7	7
38	Self-assembled films from chitosan and poly(vinyl sulfonic acid) on Nafion [®] for direct methanol fuel cell. <i>Journal of the Brazilian Chemical Society</i> , 2012, 23, 531-537.	0.6	6
39	Interaction of cyclic and linear Labaditin peptides with anionic and zwitterionic micelles. <i>Journal of Colloid and Interface Science</i> , 2015, 438, 39-46.	5.0	6
40	Development of coarse-grained force field to investigate sodium-ion transport mechanisms in cyanoborate-based ionic liquid. <i>Journal of Molecular Liquids</i> , 2021, 338, 116648.	2.3	6
41	Single-beam interface thermal lensing. <i>Applied Optics</i> , 1999, 38, 1213.	2.1	5
42	Molecular Dynamics Simulations of the Initial-State Predict Product Distributions of Dediazonation of Aryldiazonium in Binary Solvents. <i>Journal of Organic Chemistry</i> , 2015, 80, 8637-8642.	1.7	5
43	Counterion-mediated Ca ²⁺ accumulation on cationic Langmuir-Blodgett films as template for CaCO ₃ growth. <i>Thin Solid Films</i> , 2017, 638, 433-440.	0.8	5
44	Citronellal assumes a folded conformation in solution due to dispersion interactions: A joint NMR-DFT analysis. <i>Journal of Molecular Structure</i> , 2018, 1157, 401-407.	1.8	5
45	Parameterization of a coarse-grained model of cholesterol with point-dipole electrostatics. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 1259-1271.	1.3	5
46	Synergistic long-range effects of mutations underlie aggregation propensities of amylin analogues. <i>Journal of Molecular Modeling</i> , 2019, 25, 263.	0.8	5
47	In vitro enantioselective inhibition of the main human CYP450 enzymes involved in drug metabolism by the chiral pesticide tebuconazole. <i>Toxicology Letters</i> , 2021, 351, 1-9.	0.4	5
48	A simple method for the fast calculation of charge redistribution of solutes in an implicit solvent model. <i>Chemical Physics</i> , 2002, 282, 237-243.	0.9	4
49	An Explanation about the Use of (S)-Citronellal as a Chiral Derivatizing Agent (CDA) in ¹ H and ¹³ C NMR for Sec-Butylamine, Methylbenzylamine, and Amphetamine: A Theoretical-Experimental Study. <i>Molecules</i> , 2019, 24, 2830.	1.7	4
50	Computational insights into substituent effects on the stability and reactivity of flavylum cation analogs of anthocyanins. <i>Arkivoc</i> , 2020, 2020, 146-162.	0.3	2
51	Osmotic Method for Calculating Surface Pressure of Monolayers in Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2022, , .	2.3	2
52	SSPBE: um programa para solu�o num�rica da equa�o de Poisson-Boltzmann em simetria esf�rica com modelo de adsor�o. <i>Quimica Nova</i> , 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