

Renato L T Parreira

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

86

papers

673

citations

15

h-index

22

g-index

95

ext. papers

829

ext. citations

3.6

avg, IF

3.96

L-index

#	Paper	IF	Citations
86	Conformational preferences of non-nucleoside HIV-1 reverse transcriptase inhibitors. <i>Tetrahedron</i> , 2001 , 57, 3243-3253	2.4	72
85	Ureasil-poly(ethylene oxide) hybrid matrix for selective adsorption and separation of dyes from water. <i>Langmuir</i> , 2014 , 30, 3857-68	4	36
84	Characterization of hydrogen bonds in the interactions between the hydroperoxyl radical and organic acids. <i>Journal of the American Chemical Society</i> , 2003 , 125, 15614-22	16.4	31
83	The nature of the interactions between Pt ₄ cluster and the adsorbates *H, *OH, and H ₂ O. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 11731-43	2.8	29
82	On the origin of red and blue shifts of X-H and C-H stretching vibrations in formic acid (formate ion) and proton donor complexes. <i>ChemPhysChem</i> , 2007 , 8, 87-92	3.2	27
81	Computational study of formamide-water complexes using the SAPT and AIM methods. <i>Chemical Physics</i> , 2006 , 331, 96-110	2.3	27
80	How the electron-deficient cavity of heterocalixarenes recognizes anions: insights from computation. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 24696-24705	3.6	25
79	Cucurbituril-Mediated Catalytic Hydrolysis: A Kinetic and Computational Study with Neutral and Cationic Dioxolanes in CB7. <i>ACS Catalysis</i> , 2018 , 8, 12067-12079	13.1	25
78	Self-assembled films from WO ₃ : Electrochromism and lithium ion diffusion. <i>Electrochemistry Communications</i> , 2010 , 12, 733-736	5.1	22
77	Isatin-Schiff base copper(II) complexes: A DFT study of the metal-ligand bonding situation. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 625-646	2.1	21
76	Anion Recognition by Organometallic Calixarenes: Analysis from Relativistic DFT Calculations. <i>Organometallics</i> , 2018 , 37, 2167-2176	3.8	20
75	Tuning Heterocalixarenes to Improve Their Anion Recognition: A Computational Approach. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 3328-3336	2.8	19
74	Ru-NO and Ru-NO ₂ bonding linkage isomerism in cis-[Ru(NO)(NO)(bpy) ₂](2+/+) complexes - a theoretical insight. <i>Dalton Transactions</i> , 2014 , 43, 8792-804	4.3	18
73	Copaifera duckei Oleoresin and Its Main Nonvolatile Terpenes: In Vitro Schistosomicidal Properties. <i>Chemistry and Biodiversity</i> , 2016 , 13, 1348-1356	2.5	16
72	A route to obtain Gd ₂ O ₃ :Nd ³⁺ with different particle size. <i>Materials Chemistry and Physics</i> , 2011 , 127, 40-44	4.4	16
71	Computational study of pyrylium cation-water complexes: hydrogen bonds, resonance effects, and aromaticity. <i>Computational and Theoretical Chemistry</i> , 2006 , 760, 59-73		15
70	The two faces of hydrogen-bond strength on triple AAA-DDD arrays. <i>ChemPhysChem</i> , 2013 , 14, 3994-4001	3.12	13

69	In vitro cytotoxicity and structure-activity relationship approaches of ent-kaurenoic acid derivatives against human breast carcinoma cell line. <i>Phytochemistry</i> , 2018 , 156, 214-223	4	13
68	Shedding Light on the Nature of Host-Guest Interactions in PAHs-ExBox4+ Complexes. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 15480-15487	3.8	12
67	CO, NO, and SO adsorption on Ni nanoclusters: a DFT investigation. <i>Dalton Transactions</i> , 2020 , 49, 6407-6417	4.5	12
66	Biotransformation of ent-pimaradienoic acid by cell cultures of <i>Aspergillus niger</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2013 , 21, 5870-5	3.4	11
65	A novel hybrid organic-inorganic silsesquioxane and cobalt(II) tetrasulphophthalocyanine material as an efficient electrochemical sensor for the simultaneous determination of the anti-hypertensive nifedipine and its metabolite. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 6839-6850	7.1	11
64	In vivo and in silico anti-inflammatory mechanism of action of the semisynthetic (-)-cubebin derivatives (-)-hinokinin and (-)-O-benzylcubebin. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2017 , 27, 176-179	2.9	10
63	The ability of Ex2Box4+ to interact with guests containing Eelectron-rich and Eelectron-poor moieties. <i>International Journal of Quantum Chemistry</i> , 2018 , 118, e25607	2.1	9
62	Silver Nanoparticles-Silsesquioxane Nanomaterial Applied to the Determination of 4-Nitrophenol as a Biomarker. <i>Electroanalysis</i> , 2019 , 31, 2319-2329	3	9
61	(E)-Licarin A and its semi-synthetic derivatives: In vitro and in silico evaluation of trypanocidal and schistosomicidal activities. <i>Acta Tropica</i> , 2020 , 202, 105248	3.2	9
60	Quest for Insight into Ultrashort C-H...Proximities in Molecular "Iron Maidens". <i>Journal of Organic Chemistry</i> , 2018 , 83, 5114-5122	4.2	7
59	Gas-phase fragmentation reactions of protonated cocaine: New details to an old story. <i>Journal of Mass Spectrometry</i> , 2018 , 53, 203-213	2.2	7
58	Electronic properties and metal-ligand bonding situation in Eu(III) complexes containing tris(pyrazolyl)borate and phenantroline ligands. <i>Journal of Luminescence</i> , 2017 , 182, 137-145	3.8	7
57	Bond Analysis in DihalogenHalide and DihalogenDimethylchalcogenide Systems. <i>European Journal of Inorganic Chemistry</i> , 2018 , 2018, 1007-1015	2.3	6
56	Hydrazine decomposition on a small platinum cluster: the role of N2H5 intermediate. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	6
55	A theoretical indicator of transition-metal nanoclusters applied in the carbon nanotube nucleation process: a DFT study. <i>Dalton Transactions</i> , 2020 , 49, 492-503	4.3	6
54	Ruthenium nitrosyl complexes containing pyridine-functionalized carbenes I A theoretical insight. <i>Journal of Organometallic Chemistry</i> , 2015 , 799-800, 54-60	2.3	5
53	Helicenes as Molecular Tweezers in the Formation of Cation-I Complexes. Bonding and Circular Dichroism Properties from Relativistic DFT Calculations. <i>ChemPhysChem</i> , 2018 , 19, 2321-2330	3.2	5
52	Platinum nanoparticles embedded in layer-by-layer films from SnO2/polyallylamine for ethanol electrooxidation. <i>Journal of Power Sources</i> , 2008 , 185, 6-12	8.9	5

51	The usefulness of energy decomposition schemes to rationalize host-guest interactions. <i>Dalton Transactions</i> , 2020 , 49, 17457-17471	4.3	5
50	On the cation- π capabilities of small all sp^2 -carbon host structures. Evaluation of [6.8]3cyclacene from relativistic DFT calculations. <i>International Journal of Quantum Chemistry</i> , 2019 , 119, e25811	2.1	5
49	How Do Secondary Phosphine Oxides Interact with Silver Nanoclusters? Insights from Computation. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 21449-21461	3.8	5
48	Licochalcone a Exhibits Leishmanicidal Activity and in Experimental Model of (). <i>Frontiers in Veterinary Science</i> , 2020 , 7, 527	3.1	4
47	Evaluation of Electron Donation as a Mechanism for the Stabilisation of Chalcogenate-Protected Gold Nanoclusters. <i>ChemPhysChem</i> , 2016 , 17, 3102-3111	3.2	4
46	Transport properties of ruthenophanes Δ theoretical insight. <i>Chemical Physics</i> , 2016 , 478, 23-33	2.3	4
45	Removal of the emerging contaminant bisphenol A by an ureasil-PEO hybrid membrane: experimental study and molecular dynamic simulation. <i>Environmental Science and Pollution Research</i> , 2017 , 24, 18421-18433	5.1	4
44	Hydrogen bond and the resonance effect on the formamide-water complexes. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 1401-1420	2.1	4
43	How does the acidic milieu interfere in the capability of ruthenium nitrosyl complexes to release nitric oxide?. <i>New Journal of Chemistry</i> , 2020 , 44, 773-779	3.6	4
42	Schistosomicidal activity of kaurane, labdane and clerodane-type diterpenes obtained by fungal transformation. <i>Process Biochemistry</i> , 2020 , 98, 34-40	4.8	4
41	Evaluation of Lignans from Piper cubeba against Schistosoma mansoni Adult Worms: A Combined Experimental and Theoretical Study. <i>Chemistry and Biodiversity</i> , 2019 , 16, e1800305	2.5	4
40	In Silico Design of Cylindrophanes: The Role of Functional Groups in a Fluoride Selective Host. <i>ChemPhysChem</i> , 2020 , 21, 1989-2005	3.2	3
39	Understanding the interplay between π - π and cation- π interactions in [janusene-Ag] host-guest systems: a computational approach. <i>Dalton Transactions</i> , 2019 , 48, 13281-13292	4.3	3
38	Resonance in compounds with multiple conjugated bonds. <i>Structural Chemistry</i> , 2013 , 24, 1153-1162	1.8	3
37	On the recognition of chloride, bromide and nitrate anions by anthracene-quaramide conjugated compounds: a computational perspective. <i>New Journal of Chemistry</i> , 2020 , 44, 17831-17839	3.6	3
36	Kinetics and adsorption calculations: insights into the MgO-catalyzed detoxification of simulants of organophosphorus biocides. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 19011-19021	13	3
35	Metal-ligand bonding situation in ruthenophanes containing i,j-xylylene-linked bis(NHC)cyclophane ligands. <i>Journal of Organometallic Chemistry</i> , 2017 , 830, 100-108	2.3	2
34	Tracking the role of trans-ligands in ruthenium-NO bond lability: computational insight. <i>New Journal of Chemistry</i> , 2020 , 44, 11448-11456	3.6	2

33	Fungal biocatalysts for labdane diterpene hydroxylation. <i>Bioprocess and Biosystems Engineering</i> , 2020 , 43, 1051-1059	3.7	2
32	Copaifera multijuga, Copaifera pubiflora and Copaifera trapezifolia Oleoresins: Chemical Characterization and in vitro Cytotoxic Potential against Tumoral Cell Lines. <i>Journal of the Brazilian Chemical Society</i> ,	1.5	2
31	What is the driving force behind molecular triangles and their guests? A quantum chemical perspective about host-guest interactions. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 19213-19222	3.6	2
30	Evaluation of the antiseptic and wound healing potential of polyhexamethylene guanidine hydrochloride as well as its toxic effects. <i>European Journal of Pharmaceutical Sciences</i> , 2021 , 160, 105739 ^{5.1}	5.1	2
29	Bare versus protected tetrairidium clusters by density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 29480-29492	3.6	2
28	Supersaturating drug delivery systems containing fixed-dose combination of two antihypertensive drugs: Formulation, in vitro evaluation and molecular metadynamics simulations. <i>European Journal of Pharmaceutical Sciences</i> , 2021 , 163, 105860	5.1	2
27	Solvation Enhances the Distinction between Carboxylated Armchair and Zigzag Single-Wall Carbon Nanotubes (SWNT-COOH). <i>Journal of Physical Chemistry C</i> , 2017 , 121, 9516-9527	3.8	1
26	The anionic recognition mechanism based on polyol and boronic acid receptors. <i>New Journal of Chemistry</i> , 2020 , 44, 5564-5571	3.6	1
25	Electrospray ionization tandem mass spectrometry of monoketone curcuminoids. <i>Rapid Communications in Mass Spectrometry</i> , 2020 , 34 Suppl 3, e8699	2.2	1
24	Shedding light on the bonding situation of triangular and square heterometallic clusters: computational insight. <i>New Journal of Chemistry</i> , 2020 , 44, 5079-5087	3.6	1
23	Tracking the absence of anion interactions in modified [23](1,3,5)cyclophanes: insights from computation. <i>New Journal of Chemistry</i> , 2019 , 43, 13271-13281	3.6	1
22	Pt/TiO ₂ /poly(vinyl sulfonic acid) layer-by-layer films for methanol electrocatalytic oxidation. <i>Journal of Nanoscience and Nanotechnology</i> , 2009 , 9, 6620-6	1.3	1
21	The bonding situation in heteromultimetallic carbonyl complexes. <i>Dalton Transactions</i> , 2020 , 49, 16762-16771	4.9	1
20	Synthesis and luminescent properties of new naphthoquinoline lactone derivatives. <i>Journal of Luminescence</i> , 2020 , 227, 117547	3.8	1
19	Stability Changes in Iridium Nanoclusters via Monoxide Adsorption: A DFT Study within the van der Waals Corrections. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 4805-4818	2.8	1
18	Green and Red Brazilian Propolis: Antimicrobial Potential and Anti-Virulence against ATCC and Clinically Isolated Multidrug-Resistant Bacteria. <i>Chemistry and Biodiversity</i> , 2021 , 18, e2100307	2.5	1
17	Can the relative positions (cis/trans) of ligands really modulate the coordination of NO in ruthenium nitrosyl complexes?. <i>New Journal of Chemistry</i> , 2021 , 45, 1658-1666	3.6	1
16	The design of anion interactions and hydrogen bonds for the recognition of chloride, bromide and nitrate anions. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 11455-11465	3.6	1

15	Double-bond elucidation for arsagermene with a tricoordinate germanium center: a theoretical survey. <i>New Journal of Chemistry</i> , 2019 , 43, 15681-15690	3.6	o
14	Structural investigation of group 10 metal complexes with thiosemicarbazone: crystal structure, mass spectrometry, Hirshfeld surface and in vitro antitumor activity. <i>Structural Chemistry</i> , 2020 , 31, 2093-2103	1.8	o
13	Study of Anti-Tuberculosis Activity Behaviour of Natural Kaurane and Trachylobane Diterpenes Compared with Structural Properties Obtained by Theoretical Calculations. <i>Natural Product Communications</i> , 2017 , 12, 1934578X1701200	0.9	o
12	Electrochemical, theoretical, and analytical investigation of the phenylurea herbicide fluometuron at a glassy carbon electrode. <i>Electrochimica Acta</i> , 2022 , 408, 139945	6.7	o
11	and cytotoxicity of hinokinin-loaded PLGA microparticle systems against tumoral SiHa cells. <i>Natural Product Research</i> , 2021 , 1-8	2.3	o
10	The simultaneous recognition mechanism of cations and anions using macrocyclic-iodine structures: insights from dispersion-corrected DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 23793-23803	3.6	o
9	In Vivo and in Silico Trypanocidal Activity Evaluation of (-)-Cubebin Encapsulated in PLGA Microspheres as Potential Treatment in Acute Phase. <i>Chemistry and Biodiversity</i> , 2021 , 18, e2100052	2.5	o
8	Anti-melanoma effect of ruthenium(II)-diphosphine complexes containing naphthoquinone ligand. <i>Journal of Inorganic Biochemistry</i> , 2021 , 222, 111497	4.2	o
7	Evaluation of lignan-loaded poly(ϵ -caprolactone) nanoparticles: synthesis, characterization, and schistosomicidal activity.. <i>Natural Product Research</i> , 2021 , 1-7	2.3	o
6	Are DFT Methods Able to Predict Reduction Potentials of Ruthenium Nitrosyl Complexes Accurately?. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 6186-6192	2.8	
5	Nature of hydride and halide encapsulation in Ag cages: insights from the structure and interaction energy of [Ag(X){SP(OPr)}] (X = H, F, Cl, Br, I) from relativistic DFT calculations.. <i>Physical Chemistry Chemical Physics</i> , 2021 , 24, 452-458	3.6	
4	Theoretical study of chloride complexes with hybrid macrocycles. <i>New Journal of Chemistry</i> , 2021 , 45, 463-470	3.6	
3	Designing boron and metal complexes for fluoride recognition: a computational perspective. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 22768-22778	3.6	
2	The donor/acceptor trans effect on NO release in ruthenium nitrosyl complexes: a computational insight. <i>New Journal of Chemistry</i> , 2021 , 45, 8949-8957	3.6	
1	Baccharin from Brazilian green propolis induces neurotrophic signaling pathways in PC12 cells: potential for axonal and synaptic regeneration.. <i>Naunyn-Schmiedeberg's Archives of Pharmacology</i> , 2022 , 395, 659	3.4	