Renato L T Parreira

List of Publications by Year in Descending Order

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	Electrochemical, theoretical, and analytical investigation of the phenylurea herbicide fluometuron at a glassy carbon electrode. *Electrochimica Acta*, **2022**, 408, 139945	6.7	0
85	Baccharin from Brazilian green propolis induces neurotrophic signaling pathways in PC12 cells: potential for axonal and synaptic regeneration.. *Naunyn-Schmiedeberg's Archives of Pharmacology*, **2022**, 395, 659	3.4	
84	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.. *Physical Chemistry Chemical Physics*, **2021**, 24, 452-458	3.6	
83	and cytotoxicity of hinokinin-loaded PLGA microparticle systems against tumoral SiHa cells. *Natural Product Research*, **2021**, 1-8	2.3	0
82	In Vivo and in Silico Trypanocidal Activity Evaluation of (-)-Cubebin Encapsulated in PLGA Microspheres as Potential Treatment in Acute Phase. *Chemistry and Biodiversity*, **2021**, 18, e2100052	2.5	0
81	Evaluation of the antiseptic and wound healing potential of polyhexamethylene guanidine hydrochloride as well as its toxic effects. *European Journal of Pharmaceutical Sciences*, **2021**, 160, 105739	5.1	2
80	Stability Changes in Iridium Nanoclusters via Monoxide Adsorption: A DFT Study within the van der Waals Corrections. *Journal of Physical Chemistry A*, **2021**, 125, 4805-4818	2.8	1
79	Green and Red Brazilian Propolis: Antimicrobial Potential and Anti-Virulence against ATCC and Clinically Isolated Multidrug-Resistant Bacteria. *Chemistry and Biodiversity*, **2021**, 18, e2100307	2.5	1
78	Theoretical study of chloride complexes with hybrid macrocycles. *New Journal of Chemistry*, **2021**, 45, 463-470	3.6	
77	Can the relative positions (cis trans) of ligands really modulate the coordination of NO in ruthenium nitrosyl complexes?. *New Journal of Chemistry*, **2021**, 45, 1658-1666	3.6	1
76	The design of anion- interactions and hydrogen bonds for the recognition of chloride, bromide and nitrate anions. *Physical Chemistry Chemical Physics*, **2021**, 23, 11455-11465	3.6	1
75	Designing boron and metal complexes for fluoride recognition: a computational perspective. *Physical Chemistry Chemical Physics*, **2021**, 23, 22768-22778	3.6	
74	The donor/acceptor trans effect on NO release in ruthenium nitrosyl complexes: a computational insight. *New Journal of Chemistry*, **2021**, 45, 8949-8957	3.6	
73	Supersaturating drug delivery systems containing fixed-dose combination of two antihypertensive drugs: Formulation, in vitro evaluation and molecular metadynamics simulations. *European Journal of Pharmaceutical Sciences*, **2021**, 163, 105860	5.1	2
72	Anti-melanoma effect of ruthenium(II)-diphosphine complexes containing naphthoquinone ligand. *Journal of Inorganic Biochemistry*, **2021**, 222, 111497	4.2	0
71	Evaluation of lignan-loaded poly(caprolactone) nanoparticles: synthesis, characterization, and schistosomicidal activity.. *Natural Product Research*, **2021**, 1-7	2.3	0
70	Licochalcone a Exhibits Leishmanicidal Activity and in Experimental Model of (). *Frontiers in Veterinary Science*, **2020**, 7, 527	3.1	4

69	Tracking the role of trans-ligands in ruthenium–NO bond lability: computational insight. *New Journal of Chemistry*, **2020**, 44, 11448-11456	3.6	2
68	In Silico Design of Cylindrophanes: The Role of Functional Groups in a Fluoride Selective Host. *ChemPhysChem*, **2020**, 21, 1989-2005	3.2	3
67	The anionic recognition mechanism based on polyol and boronic acid receptors. *New Journal of Chemistry*, **2020**, 44, 5564-5571	3.6	1
66	Fungal biocatalysts for labdane diterpene hydroxylation. *Bioprocess and Biosystems Engineering*, **2020**, 43, 1051-1059	3.7	2
65	Are DFT Methods Able to Predict Reduction Potentials of Ruthenium Nitrosyl Complexes Accurately?. *Journal of Physical Chemistry A*, **2020**, 124, 6186-6192	2.8	
64	Structural investigation of group 10 metal complexes with thiosemicarbazone: crystal structure, mass spectrometry, Hirshfeld surface and in vitro antitumor activity. *Structural Chemistry*, **2020**, 31, 2093-2103	1.8	0
63	Electrospray ionization tandem mass spectrometry of monoketone curcuminoids. *Rapid Communications in Mass Spectrometry*, **2020**, 34 Suppl 3, e8699	2.2	1
62	Shedding light on the bonding situation of triangular and square heterometallic clusters: computational insight. *New Journal of Chemistry*, **2020**, 44, 5079-5087	3.6	1
61	(±)-Licarin A and its semi-synthetic derivatives: In vitro and in silico evaluation of trypanocidal and schistosomicidal activities. *Acta Tropica*, **2020**, 202, 105248	3.2	9
60	How does the acidic milieu interfere in the capability of ruthenium nitrosyl complexes to release nitric oxide?. *New Journal of Chemistry*, **2020**, 44, 773-779	3.6	4
59	A theoretical indicator of transition-metal nanoclusters applied in the carbon nanotube nucleation process: a DFT study. *Dalton Transactions*, **2020**, 49, 492-503	4.3	6
58	The bonding situation in heteromultimetallic carbonyl complexes. *Dalton Transactions*, **2020**, 49, 16762-16771	4.3	1
57	The simultaneous recognition mechanism of cations and anions using macrocyclic-iodine structures: insights from dispersion-corrected DFT calculations. *Physical Chemistry Chemical Physics*, **2020**, 22, 23795-23803	3.6	9
56	The usefulness of energy decomposition schemes to rationalize host-guest interactions. *Dalton Transactions*, **2020**, 49, 17457-17471	4.3	5
55	What is the driving force behind molecular triangles and their guests? A quantum chemical perspective about host-guest interactions. *Physical Chemistry Chemical Physics*, **2020**, 22, 19213-19222	3.6	2
54	Synthesis and luminescent properties of new naphthoquinoline lactone derivatives. *Journal of Luminescence*, **2020**, 227, 117547	3.8	1
53	Schistosomicidal activity of kaurane, labdane and clerodane-type diterpenes obtained by fungal transformation. *Process Biochemistry*, **2020**, 98, 34-40	4.8	4
52	On the recognition of chloride, bromide and nitrate anions by anthracene–squaramide conjugated compounds: a computational perspective. *New Journal of Chemistry*, **2020**, 44, 17831-17839	3.6	3

51	Kinetics and adsorption calculations: insights into the MgO-catalyzed detoxification of simulants of organophosphorus biocides. *Journal of Materials Chemistry A*, **2020**, 8, 19011-19021	13	3
50	CO, NO, and SO adsorption on Ni nanoclusters: a DFT investigation. *Dalton Transactions*, **2020**, 49, 6407-6417	4.5	12
49	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. *Journal of Materials Chemistry C*, **2020**, 8, 6839-6850	7.1	11
48	Double-bond elucidation for arsagermene with a tricoordinate germanium center: a theoretical survey. *New Journal of Chemistry*, **2019**, 43, 15681-15690	3.6	0
47	Tracking the absence of anion–π interactions in modified [23](1,3,5)cyclophanes: insights from computation. *New Journal of Chemistry*, **2019**, 43, 13271-13281	3.6	1
46	Understanding the interplay between π and cation–π interactions in [janusene-Ag] host-guest systems: a computational approach. *Dalton Transactions*, **2019**, 48, 13281-13292	4.3	3
45	Silver Nanoparticles-Silsesquioxane Nanomaterial Applied to the Determination of 4-Nitrophenol as a Biomarker. *Electroanalysis*, **2019**, 31, 2319-2329	3	9
44	On the cation–π capabilities of small all sp2-carbon host structures. Evaluation of [6.8]3cyclacene from relativistic DFT calculations. *International Journal of Quantum Chemistry*, **2019**, 119, e25811	2.1	5
43	Evaluation of Lignans from Piper cubeba against Schistosoma mansoni Adult Worms: A Combined Experimental and Theoretical Study. *Chemistry and Biodiversity*, **2019**, 16, e1800305	2.5	4
42	Quest for Insight into Ultrashort C-H···π Proximities in Molecular "Iron Maidens". *Journal of Organic Chemistry*, **2018**, 83, 5114-5122	4.2	7
41	The ability of Ex2Box4+ to interact with guests containing π-electron-rich and π-electron-poor moieties. *International Journal of Quantum Chemistry*, **2018**, 118, e25607	2.1	9
40	Bond Analysis in Dihalogen–Halide and Dihalogen–Dimethylchalcogenide Systems. *European Journal of Inorganic Chemistry*, **2018**, 2018, 1007-1015	2.3	6
39	Gas-phase fragmentation reactions of protonated cocaine: New details to an old story. *Journal of Mass Spectrometry*, **2018**, 53, 203-213	2.2	7
38	Tuning Heterocalixarenes to Improve Their Anion Recognition: A Computational Approach. *Journal of Physical Chemistry A*, **2018**, 122, 3328-3336	2.8	19
37	Helicenes as Molecular Tweezers in the Formation of Cation–π Complexes. Bonding and Circular Dichroism Properties from Relativistic DFT Calculations. *ChemPhysChem*, **2018**, 19, 2321-2330	3.2	5
36	Bare versus protected tetrairidium clusters by density functional theory. *Physical Chemistry Chemical Physics*, **2018**, 20, 29480-29492	3.6	2
35	Cucurbituril-Mediated Catalytic Hydrolysis: A Kinetic and Computational Study with Neutral and Cationic Dioxolanes in CB7. *ACS Catalysis*, **2018**, 8, 12067-12079	13.1	25
34	In vitro cytotoxicity and structure-activity relationship approaches of ent-kaurenoic acid derivatives against human breast carcinoma cell line. *Phytochemistry*, **2018**, 156, 214-223	4	13

33	How Do Secondary Phosphine Oxides Interact with Silver Nanoclusters? Insights from Computation. *Journal of Physical Chemistry C*, **2018**, 122, 21449-21461	3.8	5
32	Anion Recognition by Organometallic Calixarenes: Analysis from Relativistic DFT Calculations. *Organometallics*, **2018**, 37, 2167-2176	3.8	20
31	Solvation Enhances the Distinction between Carboxylated Armchair and Zigzag Single-Wall Carbon Nanotubes (SWNT-COOH). *Journal of Physical Chemistry C*, **2017**, 121, 9516-9527	3.8	1
30	In vivo and in silico anti-inflammatory mechanism of action of the semisynthetic (-)-cubebin derivatives (-)-hinokinin and (-)-O-benzylcubebin. *Bioorganic and Medicinal Chemistry Letters*, **2017**, 27, 176-179	2.9	10
29	Metal-ligand bonding situation in ruthenophanes containing i,j-xylylene-linked bis(NHC)cyclophane ligands. *Journal of Organometallic Chemistry*, **2017**, 830, 100-108	2.3	2
28	Removal of the emerging contaminant bisphenol A by an ureasil-PEO hybrid membrane: experimental study and molecular dynamic simulation. *Environmental Science and Pollution Research*, **2017**, 24, 18421-18433	5.1	4
27	How the electron-deficient cavity of heterocalixarenes recognizes anions: insights from computation. *Physical Chemistry Chemical Physics*, **2017**, 19, 24696-24705	3.6	25
26	Electronic properties and metal-ligand bonding situation in Eu(III) complexes containing tris(pyrazolyl)borate and phenantroline ligands. *Journal of Luminescence*, **2017**, 182, 137-145	3.8	7
25	Study of Anti-Tuberculosis Activity Behaviour of Natural Kaurane and Trachylobane Diterpenes Compared with Structural Properties Obtained by Theoretical Calculations. *Natural Product Communications*, **2017**, 12, 1934578X1701200	0.9	0
24	Copaifera duckei Oleoresin and Its Main Nonvolatile Terpenes: In Vitro Schistosomicidal Properties. *Chemistry and Biodiversity*, **2016**, 13, 1348-1356	2.5	16
23	Evaluation of Electron Donation as a Mechanism for the Stabilisation of Chalcogenate-Protected Gold Nanoclusters. *ChemPhysChem*, **2016**, 17, 3102-3111	3.2	4
22	Shedding Light on the Nature of Host□Guest Interactions in PAHs-ExBox4+ Complexes. *Journal of Physical Chemistry C*, **2016**, 120, 15480-15487	3.8	12
21	Transport properties of ruthenophanes □A theoretical insight. *Chemical Physics*, **2016**, 478, 23-33	2.3	4
20	Hydrazine decomposition on a small platinum cluster: the role of N2H5 intermediate. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	6
19	Ruthenium nitrosyl complexes containing pyridine-functionalized carbenes □A theoretical insight. *Journal of Organometallic Chemistry*, **2015**, 799-800, 54-60	2.3	5
18	Ru-NO and Ru-NO2 bonding linkage isomerism in cis-[Ru(NO)(NO)(bpy)2](2+/+) complexes - a theoretical insight. *Dalton Transactions*, **2014**, 43, 8792-804	4.3	18
17	Ureasil-poly(ethylene oxide) hybrid matrix for selective adsorption and separation of dyes from water. *Langmuir*, **2014**, 30, 3857-68	4	36
16	Biotransformation of ent-pimaradienoic acid by cell cultures of Aspergillus niger. *Bioorganic and Medicinal Chemistry*, **2013**, 21, 5870-5	3.4	11

15	Resonance in compounds with multiple conjugated bonds. *Structural Chemistry*, **2013**, 24, 1153-1162	1.8	3
14	The two faces of hydrogen-bond strength on triple AAA-DDD arrays. *ChemPhysChem*, **2013**, 14, 3994-4001	3.2	13
13	Isatin-Schiff base copper(II) complexes: A DFT study of the metal-ligand bonding situation. *International Journal of Quantum Chemistry*, **2012**, 112, 625-646	2.1	21
12	Hydrogen bond and the resonance effect on the formamide–water complexes. *International Journal of Quantum Chemistry*, **2012**, 112, 1401-1420	2.1	4
11	A route to obtain Gd2O3:Nd3+ with different particle size. *Materials Chemistry and Physics*, **2011**, 127, 40-44	4.4	16
10	Self-assembled films from WO3: Electrochromism and lithium ion diffusion. *Electrochemistry Communications*, **2010**, 12, 733-736	5.1	22
9	Pt/TiO2/poly(vinyl sulfonic acid) layer-by-layer films for methanol electrocatalytic oxidation. *Journal of Nanoscience and Nanotechnology*, **2009**, 9, 6620-6	1.3	1
8	The nature of the interactions between Pt4 cluster and the adsorbates *H, *OH, and H2O. *Journal of Physical Chemistry A*, **2008**, 112, 11731-43	2.8	29
7	Platinum nanoparticles embedded in layer-by-layer films from SnO2/polyallylamine for ethanol electrooxidation. *Journal of Power Sources*, **2008**, 185, 6-12	8.9	5
6	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. *ChemPhysChem*, **2007**, 8, 87-92	3.2	27
5	Computational study of formamide–water complexes using the SAPT and AIM methods. *Chemical Physics*, **2006**, 331, 96-110	2.3	27
4	Computational study of pyrylium cation–water complexes: hydrogen bonds, resonance effects, and aromaticity. *Computational and Theoretical Chemistry*, **2006**, 760, 59-73		15
3	Characterization of hydrogen bonds in the interactions between the hydroperoxyl radical and organic acids. *Journal of the American Chemical Society*, **2003**, 125, 15614-22	16.4	31
2	Conformational preferences of non-nucleoside HIV-1 reverse transcriptase inhibitors. *Tetrahedron*, **2001**, 57, 3243-3253	2.4	72
1	Copaifera multijuga, Copaifera pubiflora and Copaifera trapezifolia Oleoresins: Chemical Characterization and in vitro Cytotoxic Potential against Tumoral Cell Lines. *Journal of the Brazilian Chemical Society*,	1.5	2