Luis A E Batista De Carvalho

List of Publications by Year
in descending order

118 papers	2,686 citations	136740 32 h-index	253896 43 g-index
125 all docs	125 docs citations	125 times ranked	3028 citing authors

#	Article	IF	Citations
1	Influence of cellulose ether polymers on ketoprofen release from hydrophilic matrix tablets. European Journal of Pharmaceutics and Biopharmaceutics, 2004, 58, 51-59.	2.0	127
2	s-cis and s-trans Conformers of formic, thioformic and dithioformic acids. An ab initio study. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 1945.	1.1	87
3	Conformational Stability of Ibuprofen: Assessed by DFT Calculations and Optical Vibrational Spectroscopy. Journal of Pharmaceutical Sciences, 2008, 97, 845-859.	1.6	87
4	Characterization of decavanadate and decaniobate solutions by Raman spectroscopy. Dalton Transactions, 2016, 45, 7391-7399.	1.6	74
5	Conformational study of ketoprofen by combined DFT calculations and Raman spectroscopy. International Journal of Pharmaceutics, 2006, 307, 56-65.	2.6	70
6	Heat-induced Bone Diagenesis Probed by Vibrational Spectroscopy. Scientific Reports, 2018, 8, 15935.	1.6	67
7	Chemotherapeutic response to cisplatin-like drugs in human breast cancer cells probed by vibrational microspectroscopy. Faraday Discussions, 2016, 187, 273-298.	1.6	65
8	Conformational and vibrational study of platinum(II) anticancer drugs: cis-diamminedichloroplatinum (II) as a case study. Journal of Chemical Physics, 2007, 127, 185104.	1.2	57
9	Guanine: A Combined Study Using Vibrational Spectroscopy and Theoretical Methods. Spectroscopy, 2012, 27, 273-292.	0.8	50
10	Burned bones tell their own stories: A review of methodological approaches to assess heat-induced diagenesis. Applied Spectroscopy Reviews, 2018, 53, 603-635.	3.4	50
11	Surface Enhanced Raman Spectroscopy for Quantitative Analysis: Results of a Large-Scale European Multi-Instrument Interlaboratory Study. Analytical Chemistry, 2020, 92, 4053-4064.	3.2	50
12	Biologic Activity of a Dinuclear Pd(II)â€“Spermine Complex Toward Human Breast Cancer. Chemical Biology and Drug Design, 2011, 77, 477-488.	1.5	48
13	Comparability of Raman Spectroscopic Configurations: A Large Scale Cross-Laboratory Study. Analytical Chemistry, 2020, 92, 15745-15756.	3.2	46
14	Conformational study of 1,2-diaminoethane by combined ab initio MO calculations and Raman spectroscopy. Journal of Molecular Structure, 1999, 482-483, 639-646.	1.8	42
15	Pt(II) vs Pd(II) Polyamine Complexes as New Anticancer Drugs: A Structure- Activity Study. Letters in Drug Design and Discovery, 2006, 3, 149-151.	0.4	42
16	A molecular view of cisplatin's mode of action: interplay with DNA bases and acquired resistance. Physical Chemistry Chemical Physics, 2015, 17, 5155-5171.	1.3	39
17	Decavanadate, decaniobate, tungstate and molybdate interactions with sarcoplasmic reticulum Ca2+-ATPase: quercetin prevents cysteine oxidation by vanadate but does not reverse ATPase inhibition. Dalton Transactions, 2012, 41, 12749.	1.6	38
18	An EXAFS Approach to the Study of Polyoxometalateâ€“Protein Interactions: The Case of Decavanadateâ€“Actin. Inorganic Chemistry, 2017, 56, 10893-10903.	1.9	38

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19	Influence of Cellulose Ether Mixtures on Ibuprofen Release: MC25, HPC and HPMC K100M. Pharmaceutical Development and Technology, 2006, 11, 213-228.	1.1	36
20	Use of Effective Core Potential Calculations for the Conformational and Vibrational Study of Platinum(II) Anticancer Drugs. cis-Diamminedichloroplatinum(II) as a Case Study. Journal of Physical Chemistry A, 2008, 112, 3253-3259.	1.1	36
21	Applying vibrational spectroscopy to the study of nucleobases â€“ adenine as a case-study. New Journal of Chemistry, 2013, 37, 2691.	1.4	36
22	Intracellular water â€“ an overlooked drug target? Cisplatin impact in cancer cells probed by neutrons. Physical Chemistry Chemical Physics, 2017, 19, 2702-2713.	1.3	36
23	Evidence of dimerization through Câ€”HÂ·Â·Â·O interactions in liquid 4-methoxybenzaldehyde from Raman spectra andab initio calculations. Journal of Raman Spectroscopy, 1997, 28, 867-872.	1.2	35
24	Effects of Carvedilol on Isolated Heart Mitochondria: Evidence for a Protonophoretic Mechanism. Biochemical and Biophysical Research Communications, 2000, 276, 82-87.	1.0	35
25	Effect of the Metal Center on the Antitumor Activity of the Analogous Dinuclear Spermine Chelates (PdCl2)2(Spermine) and (PtCl2)2(Spermine). Letters in Drug Design and Discovery, 2007, 4, 460-463.	0.4	34
26	Polymorphism in Cisplatin Anticancer Drug. Journal of Physical Chemistry B, 2013, 117, 6421-6429.	1.2	34
27	The importance of suppressing spin diffusion effects in the accurate determination of the spatial structure of a flexible molecule by nuclear Overhauser effect spectroscopy. Journal of Molecular Structure, 2016, 1106, 373-381.	1.8	34
28	Conformational studies by Raman spectroscopy and statistical analysis of gauche interactions in n-butylamine. Spectrochimica Acta Part A: Molecular Spectroscopy, 1986, 42, 589-597.	0.1	33
29	Molecular structure and properties of thioacetic acid. Computational and Theoretical Chemistry, 1990, 207, 67-83.	1.5	33
30	Study of Biogenic and Î±,Ï‰-Polyamines by Combined Inelastic Neutron Scattering and Raman Spectroscopies and by Ab Initio Molecular Orbital Calculations. Journal of Physical Chemistry A, 2002, 106, 2473-2482.	1.1	33
31	Role of Cellulose Ether Polymers on Ibuprofen Release from Matrix Tablets. Drug Development and Industrial Pharmacy, 2005, 31, 653-665.	0.9	33
32	Characterization of Pt-, Pd-spermine complexes for their effect on polyamine pathway and cisplatin resistance in A2780 ovarian carcinoma cells. Oncology Reports, 2010, 24, 15-24.	1.2	33
33	Determination of preferred conformations of ibuprofen in chloroform by 2D NOE spectroscopy. European Journal of Pharmaceutical Sciences, 2014, 65, 65-73.	1.9	33
34	Crystal clear: Vibrational spectroscopy reveals intrabone, intraskeleton, and interskeleton variation in human bones. American Journal of Physical Anthropology, 2018, 166, 296-312.	2.1	33
35	Inelastic Neutron Scattering Study of Pt II Complexes Displaying Anticancer Properties. ChemPhysChem, 2011, 12, 1334-1341.	1.0	31
36	The autooxidation process in linoleic acid screened by Raman spectroscopy. Journal of Raman Spectroscopy, 2012, 43, 1991-2000.	1.2	30

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37	A conformational study of hydroxyflavones by vibrational spectroscopy coupled to DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 109, 116-124.	2.0	29
38	A comparative ab initio MO study of internal rotations in ethylamine and n-propylamine. Computational and Theoretical Chemistry, 1990, 205, 327-351.	1.5	27
39	Potential of Bioapatite Hydroxyls for Research on Archeological Burned Bone. Analytical Chemistry, 2018, 90, 11556-11563.	3.2	27
40	Anticancer drug impact on DNA â€“ a study by neutron spectroscopy coupled with synchrotron-based FTIR and EXAFS. Physical Chemistry Chemical Physics, 2019, 21, 4162-4175.	1.3	27
41	Drugâ€“excipient interactions in ketoprofen: A vibrational spectroscopy study. Biopolymers, 2006, 82, 420-424.	1.2	26
42	Study of carvedilol by combined Raman spectroscopy andab initio MO calculations. Journal of Raman Spectroscopy, 2002, 33, 778-783.	1.2	25
43	Profiling of human burned bones: oxidising versus reducing conditions. Scientific Reports, 2021, 11, 1361.	1.6	24
44	Conformational insights and vibrational study of a promising anticancer agent: the role of the ligand in Pd(<scp>ii</scp>)â€“amine complexes. New Journal of Chemistry, 2015, 39, 6274-6283.	1.4	23
45	Rather yield than break: assessing the influence of human bone collagen content on heat-induced warping through vibrational spectroscopy. International Journal of Legal Medicine, 2016, 130, 1647-1656.	1.2	23
46	Conformational studies of n-propylamine by combined ab initio MO calculations and Raman spectroscopy. Spectrochimica Acta Part A: Molecular Spectroscopy, 1988, 44, 723-732.	0.1	22
47	Raman spectra of putrescine, spermidine and spermine polyamines and theirN-deuterated andN-ionized derivatives. Journal of Raman Spectroscopy, 2003, 34, 357-366.	1.2	22
48	Osteometrics in burned human skeletal remains by neutron and optical vibrational spectroscopy. RSC Advances, 2016, 6, 68638-68641.	1.7	21
49	Chemotherapeutic Targets in Osteosarcoma: Insights from Synchrotron-MicroFTIR and Quasi-Elastic Neutron Scattering. Journal of Physical Chemistry B, 2019, 123, 6968-6979.	1.2	21
50	Transverse Acoustic Modes of Biogenic and Î±,Ï‰-Polyamines:Â A Study by Inelastic Neutron Scattering and Raman Spectroscopies Coupled to DFT Calculations. Journal of Physical Chemistry A, 2006, 110, 12947-12954.	1.1	19
51	First analysis of ancient burned human skeletal remains probed by neutron and optical vibrational spectroscopy. Science Advances, 2019, 5, eaaw1292.	4.7	19
52	Chemosteometric regression models of heat exposed human bones to determine their preâ€burnt metric dimensions. American Journal of Physical Anthropology, 2020, 173, 734-747.	2.1	19
53	A molecular mechanics force field for conformational analysis of aliphatic acyclic amines. Structural Chemistry, 1990, 1, 533-542.	1.0	17
54	The C??C internal rotation in ?-alkyl substituted carbonyls and thiocarbonyls: CH(CH3)2C(?X)YH (X,Y? O) Tj ETQq0 0 0 rgBT /Overlock 10	1.5	17

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55	A New Look into the Mode of Action of Metal-Based Anticancer Drugs. Molecules, 2020, 25, 246.	1.7	17
56	Spectroscopic characterization and efflux pump modulation of a thiophene curcumin derivative. Journal of Molecular Structure, 2020, 1215, 128291.	1.8	17
57	The Influence of the Compression Force on Zidovudine Release from Matrix Tablets. AAPS PharmSciTech, 2010, 11, 1442-1448.	1.5	16
58	A conformational study of hydroxylated isoflavones by vibrational spectroscopy coupled with DFT calculations. Vibrational Spectroscopy, 2013, 68, 257-265.	1.2	16
59	Highly ordered luminescent calix[4]azacrown films showing an emission response selective to volatile tetrahydrofuran. Journal of Materials Chemistry C, 2014, 2, 9012-9020.	2.7	16
60	Role of intracellular water in the normal-to-cancer transition in human cellsâ€"insights from quasi-elastic neutron scattering. Structural Dynamics, 2020, 7, 054701.	0.9	16
61	Vibrational spectroscopy studies on linear polyamines. Biochemical Society Transactions, 2007, 35, 374-380.	1.6	15
62	Conformational behaviour of antioxidant chromones. A vibrational spectroscopy study. Vibrational Spectroscopy, 2012, 63, 325-337.	1.2	15
63	The CH3CH2âŠ– internal rotation in thiopropionic acid as studied by ab initio SCF-MO method. Computational and Theoretical Chemistry, 1990, 208, 109-121.	1.5	14
64	Raman spectra, conformational stability and normal coordinate analysis of ethylmethylamine. Journal of Raman Spectroscopy, 1995, 26, 653-661.	1.2	14
65	Intra- versus interchain interactions in Î±,Ï‰-polyamines: a Raman spectroscopy study. Vibrational Spectroscopy, 2004, 35, 165-171.	1.2	14
66	Conformational and vibrational study of cis-diamminedichloropalladium(ii). Physical Chemistry Chemical Physics, 2010, 12, 14309.	1.3	14
67	Calixarene functionalization of TiO2 nanoarrays: an effective strategy for enhancing the sensor versatility. Journal of Materials Chemistry A, 2018, 6, 10649-10654.	5.2	14
68	The drying process of Sarcocornia perennis: impact on nutritional and physico-chemical properties. Journal of Food Science and Technology, 2020, 57, 4443-4458.	1.4	14
69	The carbonî—¸hydrogen stretching region of the Raman spectra of 1,6-hexanediamine: N-deuteration, ionisation and temperature effects. Vibrational Spectroscopy, 2002, 29, 61-67.	1.2	13
70	Biomaterials from human bone â€“ probing organic fraction removal by chemical and enzymatic methods. RSC Advances, 2018, 8, 27260-27267.	1.7	13
71	Beyond metrics and morphology: the potential of FTIR-ATR and chemometrics to estimate age-at-death in human bone. International Journal of Legal Medicine, 2020, 134, 1905-1914.	1.2	13
72	Intracellular water as a mediator of anticancer drug action. International Reviews in Physical Chemistry, 2020, 39, 67-81.	0.9	13

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73	Conformational analysis of carbonyl and thiocarbonyl ethyl esters: The HC(?X) (X,Y = O or S) internal rotation. Journal of Computational Chemistry, 1992, 13, 799-809.	1.5	12
74	Spectroscopic and Theoretical Studies on Solid 1,2-Ethylenediamine Dihydrochloride Salt. ChemPhysChem, 2004, 5, 1837-1847.	1.0	12
75	Development and Validation of a RP-HPLC Method for the Determination of Zidovudine and Its Related Substances in Sustained-release Tablets. Analytical Sciences, 2011, 27, 283-289.	0.8	12
76	Pt(II) Complexes with Linear Diaminesâ€"Part I: Vibrational Study of Pt-Diaminopropane. Spectroscopy, 2012, 27, 403-413.	0.8	12
77	Anomalous surfaceâ€enhanced Raman scattering of aromatic aldehydes and carboxylic acids. Journal of Raman Spectroscopy, 2017, 48, 413-417.	1.2	12
78	A New Look into Cancerâ€"A Review on the Contribution of Vibrational Spectroscopy on Early Diagnosis and Surgery Guidance. Cancers, 2021, 13, 5336.	1.7	12
79	The temperature dependence of the Raman spectrum and gauche interactions of tri-N-butylamine: a conformational study. Canadian Journal of Chemistry, 1987, 65, 384-390.	0.6	11
80	Temperature-dependent intensities of Raman bands of di-n-butylamine. Journal of Raman Spectroscopy, 1987, 18, 115-118.	1.2	11
81	Biorefining Potential of Wild-Grown Arundo donax, Cortaderia selloana and Phragmites australis and the Feasibility of White-Rot Fungi-Mediated Pretreatments. Frontiers in Plant Science, 2021, 12, 679966.	1.7	11
82	Whoâ€™s Who? Discrimination of Human Breast Cancer Cell Lines by Raman and FTIR Microspectroscopy. Cancers, 2022, 14, 452.	1.7	11
83	On the Effects of Changing Gaussian Program Version and SCRF Defining Parameters: Isopropylamine as a Case Study. Bulletin of the Chemical Society of Japan, 2012, 85, 962-975.	2.0	10
84	In vitrorelease of ketoprofen from hydrophilic matrix tablets containing cellulose polymer mixtures. Drug Development and Industrial Pharmacy, 2013, 39, 1651-1662.	0.9	10
85	An inelastic neutron scattering study of dietary phenolic acids. Physical Chemistry Chemical Physics, 2014, 16, 7491-7500.	1.3	10
86	Novel platinum-based anticancer drug: a complete vibrational study. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 628-634.	0.2	10
87	Shedding light into the healthâ€beneficial properties of Corema album â€"A vibrational spectroscopy study. Journal of Raman Spectroscopy, 2020, 51, 313-322.	1.2	10
88	FTIR Screening to Elucidate Compositional Differences in Maize Recombinant Inbred Lines with Contrasting Saccharification Efficiency Yields. Agronomy, 2021, 11, 1130.	1.3	10
89	The impact of moderate heating on human bones: an infrared and neutron spectroscopy study. Royal Society Open Science, 2021, 8, 210774.	1.1	10
90	Nutraceutical properties of tamarillo fruits: A vibrational study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 252, 119501.	2.0	9

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91	Validation of the mPW1PW Quantum chemical calculations for the vibrational study of organic molecules â€“ reâ€assignment of the isopropylamine vibrational spectra. Journal of Physical Organic Chemistry, 2011, 24, 110-121.	0.9	8
92	On the Relevance of Considering the Intermolecular Interactions on the Prediction of the Vibrational Spectra of Isopropylamine. Journal of Chemistry, 2013, 2013, 1-12.	0.9	8
93	FTIR Spectroscopy and DFT Calculations to Probe the Kinetics of Î²-Carotene Thermal Degradation. Journal of Physical Chemistry A, 2019, 123, 5266-5273.	1.1	8
94	Determination of preferred conformations of mefenamic acid in DMSO by NMR spectroscopy and GIAO calculation. AIP Conference Proceedings, 2019, , .	0.3	8
95	Conformational analysis of carbonyl and thiocarbonyl esters: the HC(=X)YXXXCH(CH3)2 (X,Y = O or S) internal rotation. Computational and Theoretical Chemistry, 1992, 262, 87-103.	1.5	7
96	Ab initio MO conformational study of ethylmethylamine. Computational and Theoretical Chemistry, 1993, 282, 199-209.	1.5	7
97	Study of physiological and biochemical events leading to vitrification of Arbutus unedo L. cultured in vitro. Trees - Structure and Function, 2021, 35, 241-253.	0.9	7
98	Metallodrug-protein interaction probed by synchrotron terahertz and neutron scattering spectroscopy. Biophysical Journal, 2021, 120, 3070-3078.	0.2	7
99	Temperature- and solvent-dependent raman bands of n-propylamine-N-d2: a conformational study. Journal of Molecular Structure, 1990, 218, 105-110.	1.8	6
100	New sustained release of Zidovudine Matrix tablets â^' cytotoxicity toward Caco-2 cells. Drug Development and Industrial Pharmacy, 2013, 39, 1154-1166.	0.9	6
101	Vibrational and conformational studies of 1,3-diaminopropane and its N-deuterated and N-ionised derivatives. New Journal of Chemistry, 2017, 41, 10132-10147.	1.4	6
102	Human bone probed by neutron diffraction: the burning process. RSC Advances, 2019, 9, 36640-36648.	1.7	6
103	Looking for Minor Phenolic Compounds in Extra Virgin Olive Oils Using Neutron and Raman Spectroscopies. Antioxidants, 2021, 10, 643.	2.2	5
104	Novel Insights into Corema album Berries: Vibrational Profile and Biological Activity. Plants, 2021, 10, 1761.	1.6	5
105	Conformational analysis of dimethylethylamine: an ab initio MO study and comparison with ethylamine and ethylmethylamine. Computational and Theoretical Chemistry, 1993, 282, 211-221.	1.5	4
106	Oxygen-by-sulfur substitutions in glycine: conformational and vibrational effectsâ€Šâ€. Journal of the Chemical Society Perkin Transactions II, 1999, , 2507-2514.	0.9	4
107	Geochemical and mineralogical fingerprints to distinguish the exploited ferruginous mineralisations of Grotta della Monaca (Calabria, Italy). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 173, 704-720.	2.0	4
108	The association of osteochemometrics and bone mineral density in humans. American Journal of Physical Anthropology, 2021, 176, 434-444.	2.1	4

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109	New Insights on the Vibrational Dynamics of 2-Methoxy-, 4-Methoxy- and 4-Ethoxy-Benzaldehyde from INS Spectra and Periodic DFT Calculations. Materials, 2021, 14, 4561.	1.3	4
110	Water dynamics in human cancer and non-cancer tissues. Physical Chemistry Chemical Physics, 0, , .	1.3	4
111	Gamma scintigraphy in the analysis of ketoprofen behaviour from matrix tablets. International Journal of Pharmaceutics, 2013, 448, 298-304.	2.6	3
112	Vibrational spectroscopy to study ancient Roman funerary practices at the â€œHypogeum of the Garlandsâ€•(Italy). Scientific Reports, 2022, 12, 3707.	1.6	3
113	On the correction of calculated vibrational frequencies for the effects of the counterions â€” Î±,Ï‰-diamine dihydrochlorides. Journal of Molecular Modeling, 2015, 21, 266.	0.8	2
114	Conformational study and reassessment of the vibrational assignments for Norspermidine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 157, 227-237.	2.0	2
115	Vibrational Spectroscopy Studies on Biologically Relevant Molecules: From Anticancer Agents to Drugs of Abuse. ACS Symposium Series, 2007, , 338-363.	0.5	1
116	Comment on â€œAssessment of new DFT methods for predicting vibrational spectra and structure of cisplatin: Which density functional should we choose for studying platinum(II) complexes?â€• [Spectrochim. Acta A125 (2014) 431â€“439]. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 347.	2.0	1
117	Raman spectroscopic evidence for the inclusion of decanoate ion in trimethyl-Î²-cyclodextrin. Vibrational Spectroscopy, 2016, 85, 175-180.	1.2	1
118	Towards Neutron Scattering Identification of Olive Oilâ€™s Antioxidant Properties. Neutron News, 0, , 1-2.	0.1	0