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	Whoâ€™s Who? Discrimination of Human Breast Cancer Cell Lines by Raman and FTIR Microspectroscopy. Cancers, 2022, 14, 452.	1.7	11
2	Vibrational spectroscopy to study ancient Roman funerary practices at the â€œHypogeum of the Garlandsâ€•(Italy). Scientific Reports, 2022, 12, 3707.	1.6	3
3	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
4	Profiling of human burned bones: oxidising versus reducing conditions. Scientific Reports, 2021, 11, 1361.	1.6	24
5	The association of osteochemometrics and bone mineral density in humans. American Journal of Physical Anthropology, 2021, 176, 434-444.	2.1	4
6	Looking for Minor Phenolic Compounds in Extra Virgin Olive Oils Using Neutron and Raman Spectroscopies. Antioxidants, 2021, 10, 643.	2.2	5
7	Nutraceutical properties of tamarillo fruits: A vibrational study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 252, 119501.	2.0	9
8	FTIR Screening to Elucidate Compositional Differences in Maize Recombinant Inbred Lines with Contrasting Saccharification Efficiency Yields. Agronomy, 2021, 11, 1130.	1.3	10
9	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
10	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
11	Metallodrug-protein interaction probed by synchrotron terahertz and neutron scattering spectroscopy. Biophysical Journal, 2021, 120, 3070-3078.	0.2	7
12	Novel Insights into Corema album Berries: Vibrational Profile and Biological Activity. Plants, 2021, 10, 1761.	1.6	5
13	The impact of moderate heating on human bones: an infrared and neutron spectroscopy study. Royal Society Open Science, 2021, 8, 210774.	1.1	10
14	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
15	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
16	Comparability of Raman Spectroscopic Configurations: A Large Scale Cross-Laboratory Study. Analytical Chemistry, 2020, 92, 15745-15756.	3.2	46
17	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
18	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

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19	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
20	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
21	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
22	A New Look into the Mode of Action of Metal-Based Anticancer Drugs. Molecules, 2020, 25, 246.	1.7	17
23	Intracellular water as a mediator of anticancer drug action. International Reviews in Physical Chemistry, 2020, 39, 67-81.	0.9	13
24	Spectroscopic characterization and efflux pump modulation of a thiophene curcumin derivative. Journal of Molecular Structure, 2020, 1215, 128291.	1.8	17
25	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
26	First analysis of ancient burned human skeletal remains probed by neutron and optical vibrational spectroscopy. Science Advances, 2019, 5, eaaw1292.	4.7	19
27	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
28	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
29	Human bone probed by neutron diffraction: the burning process. RSC Advances, 2019, 9, 36640-36648.	1.7	6
30	Determination of preferred conformations of mefenamic acid in DMSO by NMR spectroscopy and GIAO calculation. AIP Conference Proceedings, 2019, , .	0.3	8
31	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
32	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
33	Novel platinum-based anticancer drug: a complete vibrational study. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 628-634.	0.2	10
34	Heat-induced Bone Diagenesis Probed by Vibrational Spectroscopy. Scientific Reports, 2018, 8, 15935.	1.6	67
35	Potential of Bioapatite Hydroxyls for Research on Archeological Burned Bone. Analytical Chemistry, 2018, 90, 11556-11563.	3.2	27
36	Biomaterials from human bone â€“ probing organic fraction removal by chemical and enzymatic methods. RSC Advances, 2018, 8, 27260-27267.	1.7	13

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37	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
38	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
39	An EXAFS Approach to the Study of Polyoxometalateâ€“Protein Interactions: The Case of Decavanadateâ€“Actin. Inorganic Chemistry, 2017, 56, 10893-10903.	1.9	38
40	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
41	Anomalous surfaceâ€enhanced Raman scattering of aromatic aldehydes and carboxylic acids. Journal of Raman Spectroscopy, 2017, 48, 413-417.	1.2	12
42	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
43	Chemotherapeutic response to cisplatin-like drugs in human breast cancer cells probed by vibrational microspectroscopy. Faraday Discussions, 2016, 187, 273-298.	1.6	65
44	Osteometrics in burned human skeletal remains by neutron and optical vibrational spectroscopy. RSC Advances, 2016, 6, 68638-68641.	1.7	21
45	Raman spectroscopic evidence for the inclusion of decanoate ion in trimethyl-Î²-cyclodextrin. Vibrational Spectroscopy, 2016, 85, 175-180.	1.2	1
46	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
47	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
48	Characterization of decavanadate and decaniobate solutions by Raman spectroscopy. Dalton Transactions, 2016, 45, 7391-7399.	1.6	74
49	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
50	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
51	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
52	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
53	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
54	An inelastic neutron scattering study of dietary phenolic acids. Physical Chemistry Chemical Physics, 2014, 16, 7491-7500.	1.3	10

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55	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
56	Determination of preferred conformations of ibuprofen in chloroform by 2D NOE spectroscopy. European Journal of Pharmaceutical Sciences, 2014, 65, 65-73.	1.9	33
57	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
58	A conformational study of hydroxylated isoflavones by vibrational spectroscopy coupled with DFT calculations. Vibrational Spectroscopy, 2013, 68, 257-265.	1.2	16
59	Applying vibrational spectroscopy to the study of nucleobases â€“ adenine as a case-study. New Journal of Chemistry, 2013, 37, 2691.	1.4	36
60	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
61	Gamma scintigraphy in the analysis of ketoprofen behaviour from matrix tablets. International Journal of Pharmaceutics, 2013, 448, 298-304.	2.6	3
62	Polymorphism in Cisplatin Anticancer Drug. Journal of Physical Chemistry B, 2013, 117, 6421-6429.	1.2	34
63	In vitrorelease of ketoprofen from hydrophilic matrix tablets containing cellulose polymer mixtures. Drug Development and Industrial Pharmacy, 2013, 39, 1651-1662.	0.9	10
64	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
65	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
66	The autooxidation process in linoleic acid screened by Raman spectroscopy. Journal of Raman Spectroscopy, 2012, 43, 1991-2000.	1.2	30
67	Conformational behaviour of antioxidant chromones. A vibrational spectroscopy study. Vibrational Spectroscopy, 2012, 63, 325-337.	1.2	15
68	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
69	Pt(II) Complexes with Linear Diaminesâ€”Part I: Vibrational Study of Pt-Diaminopropane. Spectroscopy, 2012, 27, 403-413.	0.8	12
70	Guanine: A Combined Study Using Vibrational Spectroscopy and Theoretical Methods. Spectroscopy, 2012, 27, 273-292.	0.8	50
71	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
72	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

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73	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
74	Inelastic Neutron Scattering Study of Pt II Complexes Displaying Anticancer Properties. ChemPhysChem, 2011, 12, 1334-1341.	1.0	31
75	The Influence of the Compression Force on Zidovudine Release from Matrix Tablets. AAPS PharmSciTech, 2010, 11, 1442-1448.	1.5	16
76	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
77	Conformational and vibrational study of cis-diamminedichloropalladium(ii). Physical Chemistry Chemical Physics, 2010, 12, 14309.	1.3	14
78	Conformational Stability of Ibuprofen: Assessed by DFT Calculations and Optical Vibrational Spectroscopy. Journal of Pharmaceutical Sciences, 2008, 97, 845-859.	1.6	87
79	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
80	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
81	Vibrational Spectroscopy Studies on Biologically Relevant Molecules: From Anticancer Agents to Drugs of Abuse. ACS Symposium Series, 2007, , 338-363.	0.5	1
82	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
83	Vibrational spectroscopy studies on linear polyamines. Biochemical Society Transactions, 2007, 35, 374-380.	1.6	15
84	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
85	Conformational study of ketoprofen by combined DFT calculations and Raman spectroscopy. International Journal of Pharmaceutics, 2006, 307, 56-65.	2.6	70
86	Drugâ€“excipient interactions in ketoprofen: A vibrational spectroscopy study. Biopolymers, 2006, 82, 420-424.	1.2	26
87	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
88	Influence of Cellulose Ether Mixtures on Ibuprofen Release: MC25, HPC and HPMC K100M. Pharmaceutical Development and Technology, 2006, 11, 213-228.	1.1	36
89	Role of Cellulose Ether Polymers on Ibuprofen Release from Matrix Tablets. Drug Development and Industrial Pharmacy, 2005, 31, 653-665.	0.9	33
90	Spectroscopic and Theoretical Studies on Solid 1,2-Ethylenediamine Dihydrochloride Salt. ChemPhysChem, 2004, 5, 1837-1847.	1.0	12

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91	Intra- versus interchain interactions in Î±,Ï‰-polyamines: a Raman spectroscopy study. Vibrational Spectroscopy, 2004, 35, 165-171.	1.2	14
92	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
93	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
94	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
95	Study of carvedilol by combined Raman spectroscopy andab initio MO calculations. Journal of Raman Spectroscopy, 2002, 33, 778-783.	1.2	25
96	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
97	Effects of Carvedilol on Isolated Heart Mitochondria: Evidence for a Protonophoretic Mechanism. Biochemical and Biophysical Research Communications, 2000, 276, 82-87.	1.0	35
98	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
99	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
100	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
101	Raman spectra, conformational stability and normal coordinate analysis of ethylmethylamine. Journal of Raman Spectroscopy, 1995, 26, 653-661.	1.2	14
102	Ab initio MO conformational study of ethylmethylamine. Computational and Theoretical Chemistry, 1993, 282, 199-209.	1.5	7
103	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
104	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
105	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
106	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
107	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
108	Molecular structure and properties of thioacetic acid. Computational and Theoretical Chemistry, 1990, 207, 67-83.	1.5	33

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109	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
110	A molecular mechanics force field for conformational analysis of aliphatic acyclic amines. Structural Chemistry, 1990, 1, 533-542.	1.0	17
111	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
112	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
113	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
114	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
115	Temperature-dependent intensities of Raman bands of di-n-butylamine. Journal of Raman Spectroscopy, 1987, 18, 115-118.	1.2	11
116	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
117	Towards Neutron Scattering Identification of Olive Oilâ€™s Antioxidant Properties. Neutron News, 0, , 1-2.	0.1	0
118	Water dynamics in human cancer and non-cancer tissues. Physical Chemistry Chemical Physics, 0, , .	1.3	4