

Marcia Danielle Ferreira

List of Publications by Year in descending order

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69
papers

2,081
citations

236925

25
h-index

254184

43
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71
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71
docs citations

71
times ranked

3309
citing authors

#	ARTICLE	IF	CITATIONS
1	Synthesis, biological activity, and four-dimensional quantitative structure-activity analysis of 2-arylidene indan-1,3-dione derivatives tested against <i>Daphnia magna</i> . SAR and QSAR in Environmental Research, 2021, 32, 133-150.	2.2	2
2	Control of ascorbic acid in fortified powdered soft drinks using near-infrared spectroscopy (NIRS) and multivariate analysis. Journal of Food Science and Technology, 2020, 57, 1233-1241.	2.8	5
3	Detection and discrimination of <i>Carica papaya</i> fungi through the analysis of volatile metabolites by gas chromatography and analysis of variance-principal component analysis. Journal of Chemometrics, 2020, 34, e3244.	1.3	2
4	Special issue - VIII Brazilian Chemometrics Workshop. Food Chemistry, 2019, 273, 1-2.	8.2	2
5	Influence of soil sample preparation on the quantification of NPK content via spectroscopy. Geoderma, 2019, 338, 401-409.	5.1	23
6	Synthesis of Nerol Derivatives Containing a 1,2,3-Triazole Moiety and Evaluation of Their Activities against Cancer Cell Lines. Journal of the Brazilian Chemical Society, 2018, , .	0.6	1
7	2D, 3D and Hybrid QSAR Studies of Nostoclide Analogues as Inhibitors of the Photosystem II. Journal of the Brazilian Chemical Society, 2018, , .	0.6	1
8	In vitro cytotoxicity and structure-activity relationship approaches of ent-kaurenoic acid derivatives against human breast carcinoma cell line. Phytochemistry, 2018, 156, 214-223.	2.9	21
9	<i>Bracharia plantaginea</i> as a Potential (New) Source of Shikimic Acid. Quantification by NIR and PLS Regression. Planta Medica Letters, 2017, 3, e81-e86.	0.2	2
10	Synthesis, theoretical studies, and effect on the photosynthetic electron transport of trifluoromethyl arylamides. Pest Management Science, 2017, 73, 2360-2371.	3.4	5
11	Prospective Monitoring of Bariatric Surgery: Roux-En-Y Gastric Bypass Outcomes Using Mixed-Meal Tolerance Test and Time-Resolved ¹ H NMR-Based Metabolomics. OMICS A Journal of Integrative Biology, 2016, 20, 415-423.	2.0	16
12	A best comprehension about the toxicity of phenylsulfonyl carboxylates in <i>Vibrio fischeri</i> using quantitative structure activity/property relationship methods. Journal of Hazardous Materials, 2016, 304, 233-241.	12.4	6
13	Blood Metabolome Changes Before and After Bariatric Surgery: A ¹ H NMR-Based Clinical Investigation. OMICS A Journal of Integrative Biology, 2015, 19, 318-327.	2.0	36
14	Optimized bucketing for NMR spectra: Three case studies. Chemometrics and Intelligent Laboratory Systems, 2013, 122, 93-102.	3.5	83
15	The influence of R and S configurations of a series of amphetamine derivatives on quantitative structure-activity relationship models. Analytica Chimica Acta, 2013, 759, 43-52.	5.4	18
16	Exploring in vivo violacein biosynthesis by application of multivariate curve resolution on fused UV-VIS absorption, fluorescence, and liquid chromatography-mass spectrometry data. Analytical and Bioanalytical Chemistry, 2013, 405, 1293-1302.	3.7	11
17	Exploratory and discriminative studies of commercial processed Brazilian coffees with different degrees of roasting and decaffeinated. Brazilian Journal of Food Technology, 2013, 16, 198-206.	0.8	9
18	Identification of components of Brazilian honey by ¹ H NMR and classification of its botanical origin by chemometric methods. LWT - Food Science and Technology, 2012, 49, 55-63.	5.2	87

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19	PARAFAC: Adjustment for modeling consumer study covering probiotic and conventional yogurt. Food Research International, 2012, 45, 211-215.	6.2	51
20	Digital Filters for Molecular Interaction Field Descriptors. Molecular Informatics, 2012, 31, 75-84.	2.5	15
21	Monitoring the authenticity of Brazilian UHT milk: A chemometric approach. Food Chemistry, 2011, 124, 692-695.	8.2	135
22	Multivariate QSAR study on the antimutagenic activity of flavonoids against 3-NFA on Salmonella typhimurium TA98. European Journal of Medicinal Chemistry, 2010, 45, 4562-4569.	5.5	22
23	CHEMOMETRIC STUDIES FOR QUALITY CONTROL OF PROCESSED BRAZILIAN COFFEES USING DRIFTS. Journal of Food Quality, 2010, 33, 212-227.	2.6	52
24	Theoretical Study of Acid-Catalyzed Hydrolysis of Epoxides. Journal of Physical Chemistry A, 2010, 114, 5187-5194.	2.5	27
25	Support vector regression for functional data in multivariate calibration problems. Analytica Chimica Acta, 2009, 642, 110-116.	5.4	23
26	Critical comparative analysis, validation and interpretation of SVM and PLS regression models in a QSAR study on HIV-1 protease inhibitors. Chemometrics and Intelligent Laboratory Systems, 2009, 98, 65-77.	3.5	44
27	Multivariate QSAR study of 4,5-dihydroxypyrimidine carboxamides as HIV-1 integrase inhibitors. European Journal of Medicinal Chemistry, 2009, 44, 3577-3583.	5.5	29
28	Influence of different content of cheese whey and oligofructose on the properties of fermented lactic beverages: Study using response surface methodology. LWT - Food Science and Technology, 2009, 42, 993-997.	5.2	41
29	Classification of Brazilian vinegars according to their ¹ H NMR spectra by pattern recognition analysis. LWT - Food Science and Technology, 2009, 42, 1455-1460.	5.2	53
30	Theoretical study of omeprazole behavior: Racemization barrier and decomposition reaction. International Journal of Quantum Chemistry, 2008, 108, 1097-1106.	2.0	10
31	Optimization of extraction of high-ester pectin from passion fruit peel (<i>Passiflora edulis flavicarpa</i>) with citric acid by using response surface methodology. Bioresource Technology, 2008, 99, 5561-5566.	9.6	189
32	Planilha de validação: uma nova ferramenta para estimar figuras de mérito na validação de métodos analíticos univariados. Química Nova, 2008, 31, 164-171.	0.3	73
33	Determinação de açúcar total em café cru por espectroscopia no infravermelho próximo e regressão por mínimos quadrados parciais. Química Nova, 2007, 30, 346-350.	0.3	10
34	Chemometric analysis applied in ¹ H HR-MAS NMR and FT-IR data for chemotaxonomic distinction of intact lichen samples. Analytica Chimica Acta, 2007, 595, 3-8.	5.4	31
35	Simultaneously calibrating solids, sugars and acidity of tomato products using PLS2 and NIR spectroscopy. Analytica Chimica Acta, 2007, 595, 221-227.	5.4	81
36	A study of physicochemical and biopharmaceutical properties of Amoxicillin tablets using full factorial design and PCA biplot. Analytica Chimica Acta, 2007, 595, 216-220.	5.4	10

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37	Inibidores da HIV-integrase: potencial abordagem farmacolÃ³gica para tratamento da AIDS. <i>Quimica Nova</i> , 2006, 29, 555-562.	0.3	1
38	Molecular graphics approach to bacterial AcrB proteinâ€™s lactam antibiotic molecular recognition in drug efflux mechanism. <i>Journal of Molecular Graphics and Modelling</i> , 2006, 25, 126-145.	2.4	4
39	Pattern recognition applied to mineral characterization of Brazilian coffees and sugar-cane spirits. <i>Spectrochimica Acta, Part B: Atomic Spectroscopy</i> , 2005, 60, 717-724.	2.9	65
40	QSAR model of the phototoxicity of polycyclic aromatic hydrocarbons. <i>Computational and Theoretical Chemistry</i> , 2005, 719, 191-200.	1.5	61
41	Correlation of animal diet and fatty acid content in young goat meat by gas chromatography and chemometrics. <i>Meat Science</i> , 2005, 71, 358-363.	5.5	14
42	Chemical and electrochemical properties of an Oxisolâ€™ Ultisol transition in the state of SÃ£o Paulo, Brazil. <i>Geoderma</i> , 2005, 126, 375-388.	5.1	5
43	Solid-phase spectrofluorimetric determination of acetylsalicylic acid and caffeine in pharmaceutical preparations using partial least-squares multivariate calibration. <i>Talanta</i> , 2005, 67, 65-69.	5.5	39
44	THEORETICAL AND CHEMOMETRIC STUDY OF SUBSTITUTED OXAZINES. <i>Journal of the Chilean Chemical Society</i> , 2005, 50, .	1.2	0
45	A quantum chemical and statistical study of flavonoid compounds (flavones) with anti-HIV activity. <i>European Journal of Medicinal Chemistry</i> , 2003, 38, 929-938.	5.5	22
46	QSPR models of boiling point, octanolâ€™water partition coefficient and retention time index of polycyclic aromatic hydrocarbons. <i>Computational and Theoretical Chemistry</i> , 2003, 663, 109-126.	1.5	110
47	Dual amperometric biosensor device for analysis of binary mixtures of phenols by multivariate calibration using partial least squares. <i>Analytica Chimica Acta</i> , 2003, 485, 263-269.	5.4	47
48	A priori molecular descriptors in QSAR: a case of HIV-1 protease inhibitors. <i>Journal of Molecular Graphics and Modelling</i> , 2003, 21, 435-448.	2.4	26
49	A priori molecular descriptors in QSAR: a case of HIV-1 protease inhibitors. <i>Journal of Molecular Graphics and Modelling</i> , 2003, 21, 499-515.	2.4	9
50	Spectrophotometric Determination of Caramel Content in Spirits Aged in Oak Casks. <i>Journal of AOAC INTERNATIONAL</i> , 2002, 85, 744-750.	1.5	19
51	SeleÃ§Ã£o de variÃ¡veis em QSAR. <i>Quimica Nova</i> , 2002, 25, 439-448.	0.3	43
52	Omeprazole and analogue compounds: a QSAR study of activity against <i>Helicobacter pylori</i> using theoretical descriptors. <i>Journal of Chemometrics</i> , 2002, 16, 510-520.	1.3	5
53	Structureâ€™activity relationships (SAR) of contraceptive progestogens studied with four different methods using calculated physicochemical parameters. <i>Journal of Molecular Graphics and Modelling</i> , 2002, 20, 345-358.	2.4	11
54	A multi-way analysis of starch cassava properties. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2002, 64, 123-135.	3.5	0

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55	Análise exploratória dos teores de constituintes inorgânicos em sucos e refrigerantes de uva. <i>Ecletica Quimica</i> , 2002, 27, 77-90.	0.5	11
56	Discriminação geográfica de águas minerais do Estado de São Paulo através da análise exploratória. <i>Ecletica Quimica</i> , 2002, 27, 91-102.	0.5	10
57	Polycyclic aromatic hydrocarbons: a QSPR study. <i>Chemosphere</i> , 2001, 44, 125-146.	8.2	112
58	Relationships of the minerals and fatty acid contents in processed turkey meat products. <i>Food Chemistry</i> , 2000, 69, 259-265.	8.2	33
59	Calibration and detailed analysis of second-order flow injection analysis data with rank overlap. <i>Analytica Chimica Acta</i> , 2000, 422, 21-36.	5.4	28
60	Evaluation of Phenolic Compounds in Brazilian Propolis from Different Geographic Regions. <i>Zeitschrift Fur Naturforschung - Section C Journal of Biosciences</i> , 2000, 55, 76-81.	1.4	57
61	Potassium transport through liquid membranes using spectral and chemometric methods. <i>Journal of Molecular Structure</i> , 1999, 480-481, 563-567.	3.6	3
62	Oceanographic characterization of northern São Paulo Coast: a chemometric study. <i>Chemometrics and Intelligent Laboratory Systems</i> , 1999, 47, 289-297.	3.5	15
63	Population analysis from atomic polar tensors?. <i>Journal of Molecular Structure</i> , 1993, 294, 75-78.	3.6	8
64	Ab-initio atomic charges from atomic polar tensors. <i>Journal of Molecular Structure</i> , 1992, 266, 223-228.	3.6	2
65	Interpretation of infrared intensities based on the atomic polar tensor partition. The ROH molecules (R = H, CH ₃ , NH ₂ , OH, F). <i>Journal of Molecular Structure</i> , 1990, 218, 285-289.	3.6	1
66	Infrared intensity parameters of the diacetylene and acidity of acetylenic hydrogens. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1987, 43, 345-348.	0.1	2
67	Sensory quality prediction of coffee assessed by physicochemical parameters and Multivariate model. <i>Coffee Science</i> , 0, 15, 1-11.	0.5	1
68	Quimiometria: conceitos, métodos e aplicações. , 0, , .		67
69	Traditional herbal compounds as candidates to inhibit the SARS-CoV-2 main protease: an in silico study. <i>Journal of Biomolecular Structure and Dynamics</i> , 0, , 1-14.	3.5	3