Marcia Danielle Ferreira

List of Publications by Year
in descending order

69 papers	2,081 citations	236925 25 h-index	254184 43 g-index
71 all docs	71 docs citations	71 times ranked	3309 citing authors

#	Article	IF	Citations
1	Optimization of extraction of high-ester pectin from passion fruit peel (Passiflora edulis flavicarpa) with citric acid by using response surface methodology. Bioresource Technology, 2008, 99, 5561-5566.	9.6	189
2	Monitoring the authenticity of Brazilian UHT milk: A chemometric approach. Food Chemistry, 2011, 124, 692-695.	8.2	135
3	Polycyclic aromatic hydrocarbons: a QSPR study. Chemosphere, 2001, 44, 125-146.	8.2	112
4	QSPR models of boiling point, octanolâ€“water partition coefficient and retention time index of polycyclic aromatic hydrocarbons. Computational and Theoretical Chemistry, 2003, 663, 109-126.	1.5	110
5	Identification of components of Brazilian honey by 1H NMR and classification ofÂits botanical origin by chemometric methods. LWT - Food Science and Technology, 2012, 49, 55-63.	5.2	87
6	Optimized bucketing for NMR spectra: Three case studies. Chemometrics and Intelligent Laboratory Systems, 2013, 122, 93-102.	3.5	83
7	Simultaneously calibrating solids, sugars and acidity of tomato products using PLS2 and NIR spectroscopy. Analytica Chimica Acta, 2007, 595, 221-227.	5.4	81
8	Planilha de validaÃ§Ã£o: uma nova ferramenta para estimar figuras de mÃ©rito na validaÃ§Ã£o de mÃ©todos analÃticos univariados. Quimica Nova, 2008, 31, 164-171.	0.3	73
9	Quimiometria: conceitos, mÃ©todos e aplicaÃ§Ãµes. , 0, , .		67
10	Pattern recognition applied to mineral characterization of Brazilian coffees and sugar-cane spirits. Spectrochimica Acta, Part B: Atomic Spectroscopy, 2005, 60, 717-724.	2.9	65
11	QSAR model of the phototoxicity of polycyclic aromatic hydrocarbons. Computational and Theoretical Chemistry, 2005, 719, 191-200.	1.5	61
12	Evalution of Phenolic Compounds in Brazilian Propolis from Different Geographic Regions. Zeitschrift Fur Naturforschung - Section C Journal of Biosciences, 2000, 55, 76-81.	1.4	57
13	Classification of Brazilian vinegars according to their 1H NMR spectra by pattern recognition analysis. LWT - Food Science and Technology, 2009, 42, 1455-1460.	5.2	53
14	CHEMOMETRIC STUDIES FOR QUALITY CONTROL OF PROCESSED BRAZILIAN COFFEES USING DRIFTS. Journal of Food Quality, 2010, 33, 212-227.	2.6	52
15	PARAFAC: Adjustment for modeling consumer study covering probiotic and conventional yogurt. Food Research International, 2012, 45, 211-215.	6.2	51
16	Dual amperometric biosensor device for analysis of binary mixtures of phenols by multivariate calibration using partial least squares. Analytica Chimica Acta, 2003, 485, 263-269.	5.4	47
17	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
18	SeleÃ§Ã£o de variÃ¡veis em QSAR. Quimica Nova, 2002, 25, 439-448.	0.3	43

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19	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
20	Solid-phase spectrofluorimetric determination of acetylsalicylic acid and caffeine in pharmaceutical preparations using partial least-squares multivariate calibration. Talanta, 2005, 67, 65-69.	5.5	39
21	Blood Metabolome Changes Before and After Bariatric Surgery: A¹H NMR-Based Clinical Investigation. OMICS A Journal of Integrative Biology, 2015, 19, 318-327.	2.0	36
22	Relationships of the minerals and fatty acid contents in processed turkey meat products. Food Chemistry, 2000, 69, 259-265.	8.2	33
23	Chemometric analysis applied in 1H HR-MAS NMR and FT-IR data for chemotaxonomic distinction of intact lichen samples. Analytica Chimica Acta, 2007, 595, 3-8.	5.4	31
24	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
25	Calibration and detailed analysis of second-order flow injection analysis data with rank overlap. Analytica Chimica Acta, 2000, 422, 21-36.	5.4	28
26	Theoretical Study of Acid-Catalyzed Hydrolysis of Epoxides. Journal of Physical Chemistry A, 2010, 114, 5187-5194.	2.5	27
27	A priori molecular descriptors in QSAR: a case of HIV-1 protease inhibitors. Journal of Molecular Graphics and Modelling, 2003, 21, 435-448.	2.4	26
28	Support vector regression for functional data in multivariate calibration problems. Analytica Chimica Acta, 2009, 642, 110-116.	5.4	23
29	Influence of soil sample preparation on the quantification of NPK content via spectroscopy. Geoderma, 2019, 338, 401-409.	5.1	23
30	A quantum chemical and statistical study of flavonoid compounds (flavones) with anti-HIV activity. European Journal of Medicinal Chemistry, 2003, 38, 929-938.	5.5	22
31	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
32	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
33	Spectrophotometric Determination of Caramel Content in Spirits Aged in Oak Casks. Journal of AOAC INTERNATIONAL, 2002, 85, 744-750.	1.5	19
34	The influence of R and S configurations of a series of amphetamine derivatives on quantitative structureâ€“activity relationship models. Analytica Chimica Acta, 2013, 759, 43-52.	5.4	18
35	â€œOmicsâ€•Prospective Monitoring of Bariatric Surgery: Roux-En-Y Gastric Bypass Outcomes Using Mixed-Meal Tolerance Test and Time-Resolved¹H NMR-Based Metabolomics. OMICS A Journal of Integrative Biology, 2016, 20, 415-423.	2.0	16
36	Oceanographic characterization of northern SÃ£o Paulo Coast: a chemometric study. Chemometrics and Intelligent Laboratory Systems, 1999, 47, 289-297.	3.5	15

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37	Digital Filters for Molecular Interaction Field Descriptors. Molecular Informatics, 2012, 31, 75-84.	2.5	15
38	Correlation of animal diet and fatty acid content in young goat meat by gas chromatography and chemometrics. Meat Science, 2005, 71, 358-363.	5.5	14
39	Structureâ€“activity relationships (SAR) of contraceptive progestogens studied with four different methods using calculated physicochemical parameters. Journal of Molecular Graphics and Modelling, 2002, 20, 345-358.	2.4	11
40	Exploring in vivo violacein biosynthesis by application of multivariate curve resolution on fused UVâ€“VIS absorption, fluorescence, and liquid chromatographyâ€“mass spectrometry data. Analytical and Bioanalytical Chemistry, 2013, 405, 1293-1302.	3.7	11
41	AnÃ¡lise exploratÃ³ria dos teores de constituintes inorgÃ¢nicos em sucos e refrigerantes de uva. Ecletica Quimica, 2002, 27, 77-90.	0.5	11
42	DeterminaÃ§Ã£o de aÃ§Ãºcar total em cafÃ© cru por espectroscopia no infravermelho prÃ³ximo e regressÃ£o por mÃnimos quadrados parciais. Quimica Nova, 2007, 30, 346-350.	0.3	10
43	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
44	Theoretical study of omeprazole behavior: Racemization barrier and decomposition reaction. International Journal of Quantum Chemistry, 2008, 108, 1097-1106.	2.0	10
45	DiscriminaÃ§Ã£o geogrÃ¡fica de Ã¡guas minerais do Estado de SÃ£o Paulo atravÃ©s da anÃ¡lise exploratÃ³ria. Ecletica Quimica, 2002, 27, 91-102.	0.5	10
46	A priori molecular descriptors in QSAR: a case of HIV-1 protease inhibitors. Journal of Molecular Graphics and Modelling, 2003, 21, 499-515.	2.4	9
47	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
48	Population analysis from atomic polar tensors?. Journal of Molecular Structure, 1993, 294, 75-78.	3.6	8
49	A bestâ€‹ comprehension about the toxicity of phenylsulfonyl carboxylates in Vibrio fischeri using quantitative structure activity/property relationship methods. Journal of Hazardous Materials, 2016, 304, 233-241.	12.4	6
50	Omeprazole and analogue compounds: a QSAR study of activity againstHelicobacter pylori using theoretical descriptors. Journal of Chemometrics, 2002, 16, 510-520.	1.3	5
51	Chemical and electrochemical properties of an Oxisolâ€“Ultisol transition in the state of SÃ£o Paulo, Brazil. Geoderma, 2005, 126, 375-388.	5.1	5
52	Synthesis, theoretical studies, and effect on the photosynthetic electron transport of trifluoromethyl arylamides. Pest Management Science, 2017, 73, 2360-2371.	3.4	5
53	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
54	Molecular graphics approach to bacterial AcrB proteinâ€“Î²-lactam antibiotic molecular recognition in drug efflux mechanism. Journal of Molecular Graphics and Modelling, 2006, 25, 126-145.	2.4	4

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55	Potassium transport through liquid membranes using spectral and chemometric methods. Journal of Molecular Structure, 1999, 480-481, 563-567.	3.6	3
56	Traditional herbal compounds as candidates to inhibit the SARS-CoV-2 main protease: an in silico study. Journal of Biomolecular Structure and Dynamics, 0, , 1-14.	3.5	3
57	Infrared intensity parameters of the diacetylene and acidity of acetylenic hydrogens. Spectrochimica Acta Part A: Molecular Spectroscopy, 1987, 43, 345-348.	0.1	2
58	Ab-initio atomic charges from atomic polar tensors. Journal of Molecular Structure, 1992, 266, 223-228.	3.6	2
59	Brachiaria plantaginea as a Potential (New) Source of Shikimic Acid. Quantification by NIR and PLS Regression. Planta Medica Letters, 2017, 3, e81-e86.	0.2	2
60	Special issue â€“ VIII Brazilian Chemometrics Workshop. Food Chemistry, 2019, 273, 1-2.	8.2	2
61	Detection and discrimination of <scp>Carica papaya</scp> fungi through the analysis of volatile metabolites by gas chromatography and analysis of varianceâ€principal component analysis. Journal of Chemometrics, 2020, 34, e3244.	1.3	2
62	Synthesis, biological activity, and four-dimensional quantitative structureâ€“activity analysis of 2-arylidene indan-1,3-dione derivatives tested against Daphnia magna. SAR and QSAR in Environmental Research, 2021, 32, 133-150.	2.2	2
63	Interpretation of infrared intensities based on the atomic polar tensor partition. The ROH molecules (R = H, CH3, NH2, OH, F). Journal of Molecular Structure, 1990, 218, 285-289.	3.6	1
64	Inibidores da HIV-integrase: potencial abordagem farmacolÃ³gica para tratamento da AIDS. Quimica Nova, 2006, 29, 555-562.	0.3	1
65	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
66	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
67	Sensory quality prediction of coffee assessed by physicochemical parameters and Multivariate model. Coffee Science, 0, 15, 1-11.	0.5	1
68	A multi-way analysis of starch cassava properties. Chemometrics and Intelligent Laboratory Systems, 2002, 64, 123-135.	3.5	0
69	THEORETICAL AND CHEMOMETRIC STUDY OF SUBSTITUTED OXAZINES. Journal of the Chilean Chemical Society, 2005, 50, .	1.2	0