Roy E Bruns

List of Publications by Year
in descending order

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265	6,594	159358	88477
papers	citations	30 h-index	70 g-index

275	275	275	6526
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Unavoidable failure of point charge descriptions of electronic density changes for out-of-plane distortions. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 271, 120891.	2.0	5
2	Electronic Distribution of S_N2 IRC and TS Structures: Infrared Intensities of Imaginary Frequencies. Journal of Chemical Theory and Computation, 2022, 18, 2437-2447.	2.3	4
3	Exogenous application of bioregulators in Coffea arabica beans during ripening: Investigation of UVâ€“Visible and NIR mixture design-fingerprints using AComDim-ICA. Microchemical Journal, 2022, 181, 107702.	2.3	2
4	AC/DC Analysis: Broad and Comprehensive Approach to Analyze Infrared Intensities at the Atomic Level. Journal of Physical Chemistry A, 2021, 125, 3219-3229.	1.1	5
5	Time dependent berry maturation for planting density levels in Coffea arabica L. beans: Mixture design-fingerprinting using near-infrared transmittance spectroscopy. Journal of Food Composition and Analysis, 2021, 97, 103795.	1.9	8
6	Atomic charge and atomic dipole modeling of gas-phase infrared intensities of fundamental bands for out-of-plane CH and CF bending vibrations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 251, 119393.	2.0	5
7	Topological electron density properties at critical points along aromatic rings as reactivity and regioselectivity descriptors in electrophilic substitutions. Journal of Physical Organic Chemistry, 2021, 34, e4252.	0.9	3
8	Are â€œGAPT Chargesâ€•Really Just Charges?. Journal of Chemical Information and Modeling, 2021, 61, 3881-3890.	2.5	15
9	Electrostatics Explains the Reverse Lewis Acidity of BH3 and Boron Trihalides: Infrared Intensities and a Relative Energy Gradient (REG) Analysis of IQA Energies. Journal of Physical Chemistry A, 2021, 125, 8615-8625.	1.1	7
10	Ecometabolic mixture design-fingerprints from exploratory multi-block data analysis in Coffea arabica beans from climate changes: Elevated carbon dioxide and reduced soil water availability. Food Chemistry, 2021, 362, 129716.	4.2	7
11	Authentication of carioca common bean cultivars (Phaseolus vulgaris L.) using digital image processing and chemometric tools. Food Chemistry, 2021, 364, 130349.	4.2	8
12	Irrigated and CO2 level effects on metabolism in Coffea arabica beans from mixture design â€“ near infrared fingerprints. Microchemical Journal, 2020, 152, 104276.	2.3	10
13	Factorial design fingerprint discrimination of Coffea arabica beans under elevated carbon dioxide and limited water conditions. Talanta, 2020, 209, 120591.	2.9	14
14	The main effects of elevated CO2 and soil-water deficiency on 1H NMR-based metabolic fingerprints of Coffea arabica beans by factorial and mixture design. Science of the Total Environment, 2020, 749, 142350.	3.9	12
15	Spectroscopic and Chromatographic Fingerprints for Discrimination of Specialty and Traditional Coffees by Integrated Chemometric Methods. Food Analytical Methods, 2020, 13, 2204-2212.	1.3	14
16	FT-IR biomarkers of sexual dimorphism in yerba-mate plants: Seasonal and light accessibility effects. Microchemical Journal, 2020, 158, 105329.	2.3	12
17	Revisiting the negative dipole moment derivatives of HNgX molecules. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	0
18	Variation of the Distribution of Atmospheric n-Alkanes Emitted by Different Fuelsâ€™ Combustion. Atmosphere, 2020, 11, 643.	1.0	11

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19	A tribute to Professor Ronei J. Poppi, a pioneer of multivariate calibration in South America and a prolific mentor of chemometricians in Brazil. Journal of Chemometrics, 2020, 34, e3284.	0.7	1
20	Quantum chemical intensity determinations of overlapped gas phase infrared bands. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 230, 118067.	2.0	2
21	QTAIM Atomic Charge and Polarization Parameters and Their Machine-Learning Transference among Boron-Halide Molecules. Journal of Physical Chemistry A, 2020, 124, 3407-3416.	1.1	3
22	Special issue â€“ VIII Brazilian Chemometrics Workshop. Food Chemistry, 2019, 273, 1-2.	4.2	2
23	Potential biomonitoring of atmospheric carbon dioxide in Coffea arabica leaves using near-infrared spectroscopy and partial least squares discriminant analysis. Environmental Science and Pollution Research, 2019, 26, 30356-30364.	2.7	13
24	Infrared Intensification and Hydrogen Bond Stabilization: Beyond Point Charges. Journal of Physical Chemistry A, 2019, 123, 6482-6490.	1.1	12
25	Integrated Chemometric Approach to Optimize Sample Preparation for Detecting Metabolic Changes Provoked by Abiotic Stress in Coffea arabica L. Leaf Fingerprints. Journal of the Brazilian Chemical Society, 2019, , .	0.6	2
26	Photodiode array chromatographic-spectrophotometric metabolite quantification for yerba-mate plant sexual dimorphism differentiation. Microchemical Journal, 2019, 151, 104218.	2.3	7
27	FTIR and dispersive gas phase absolute infrared intensities of hydrocarbon fundamental bands. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 214, 1-6.	2.0	7
28	Experimental mixture design solvent effects on pigment extraction and antioxidant activity from Coffea arabica L. leaves. Microchemical Journal, 2019, 146, 713-721.	2.3	45
29	Sequential mixture design optimization for divergent metabolite analysis: Enriched carbon dioxide effects on Coffea arabica L. leaves and buds. Talanta, 2019, 191, 382-389.	2.9	19
30	Environmental stress evaluation of Coffea arabica L. leaves from spectrophotometric fingerprints by PCA and OSCâ€“PLSâ€“DA. Arabian Journal of Chemistry, 2019, 12, 4251-4257.	2.3	12
31	Seasonal changes and solvent effects on fractionated functional food component yields from Mikania laevigata leaves. Food Chemistry, 2019, 273, 151-158.	4.2	14
32	Chemometric Analysis of 1H NMR Fingerprints of Coffea arabica Green Bean Extracts Cultivated under Different Planting Densities. Food Analytical Methods, 2018, 11, 1906-1914.	1.3	13
33	Atomic Polarizations, Not Charges, Determine CH Out-of-Plane Bending Intensities of Benzene Molecules. Journal of Physical Chemistry A, 2018, 122, 9833-9841.	1.1	8
34	PARAFAC HPLC-DAD metabolomic fingerprint investigation of reference and crossed coffees. Food Research International, 2018, 113, 9-17.	2.9	15
35	Probing the robustness of the charge-charge transfer-dipolar polarization model and infrared intensities. Journal of Molecular Modeling, 2018, 24, 182.	0.8	3
36	FTIR and dispersive gas phase fundamental infrared intensities of the fluorochloromethanes: Comparison with QCISD/cc-pVTZ results. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 205, 269-275.	2.0	8

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37	Mixture Design PARAFAC HPLC-DAD Metabolomic Fingerprints of Fractionated Organic and Basic Extracts from Erythrina speciosa Andrews Leaves. Chromatographia, 2018, 81, 1189-1200.	0.7	13
38	Mixed oil formulations enriched in essential fatty acids and reduced ratio of n-6/n-3. European Journal of Lipid Science and Technology, 2017, 119, 1600400.	1.0	4
39	Factorial design effects of plant density, pattern and light availability on the caffeine, chlorogenic acids, lipids, reducing sugars and ash contents of Coffea arabica L. beans and leaves. Analytical Methods, 2017, 9, 3612-3618.	1.3	14
40	Atomic polarizations necessary for coherent infrared intensity modeling with theoretical calculations. Journal of Chemical Physics, 2017, 146, 134107.	1.2	8
41	Multivariate Optimization of Chlorogenic Acid Extraction From Brazilian Coffee. Food Analytical Methods, 2017, 10, 2943-2951.	1.3	8
42	Quantum Theory of Atoms in Molecules Chargeâ€“Charge Transferâ€“Dipolar Polarization Classification of Infrared Intensities. Journal of Physical Chemistry A, 2017, 121, 8115-8123.	1.1	3
43	Effect of selenium treated broccoli on herbivory and oviposition preferences of Delia radicum and Phyllotreta spp.. Scientia Horticulturae, 2017, 225, 445-453.	1.7	10
44	Optimization of frying oil composition rich in essential fatty acids by mixture design. LWT - Food Science and Technology, 2017, 84, 795-803.	2.5	7
45	Infrared spectral evidence and DFT calculations of hydrogen-bonding and molecular structures of acetogenins. Journal of Molecular Structure, 2017, 1130, 174-180.	1.8	4
46	Irrigation and Light Access Effects on Coffea arabica L. Leaves by FTIRâ€‘Chemometric Analysis. Journal of the Brazilian Chemical Society, 2017, , .	0.6	3
47	Chemometric Analysis of UV Characteristic Profile and Infrared Fingerprint Variations ofCoffea arabicaGreen Beans under Different Space Management Treatments. Journal of the Brazilian Chemical Society, 2016, , .	0.6	1
48	Review of Experimental GAPT and Infrared Atomic Charges in Molecules. Journal of the Brazilian Chemical Society, 2016, , .	0.6	5
49	Comment on â€œPropionaldehyde infrared crossâ€“sections and band strengthsâ€•by B. KÃ¶roÄŸlu et al.. Journal of Quantitative Spectroscopy and Radiative Transfer, 2016, 179, 137-138.	1.1	0
50	Characteristic infrared intensities of carbonyl stretching vibrations. Physical Chemistry Chemical Physics, 2016, 18, 17575-17585.	1.3	17
51	Revisiting the integrated infrared intensities and atomic polar tensors of the boron trihalides. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 164, 123-127.	2.0	1
52	QTAIM-Based Characteristic Group Infrared Intensities of Amino Acids and Their Transference to Peptides. Journal of Physical Chemistry A, 2016, 120, 8387-8399.	1.1	6
53	UV-Vis spectral fingerprinting and chemometric method applied to the evaluation of Camellia sinensis leaves from different harvests. Analytical Methods, 2016, 8, 7537-7544.	1.3	10
54	Dynamic atomic contributions to infrared intensities of fundamental bands. Physical Chemistry Chemical Physics, 2015, 17, 30378-30388.	1.3	16

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55	Multivariate optimisation of ICP OES instrumental parameters for Pb/Ba/Sb measurement in gunshot residues. Microchemical Journal, 2015, 120, 58-63.	2.3	28
56	Spectroscopic and Chromatographic Fingerprint Analysis of Composition Variations inCoffea arabicaLeaves Subject to Different Light Conditions and Plant Phenophases. Journal of the Brazilian Chemical Society, 2014, , .	0.6	3
57	Determination of Flavanones in Orange Juices Obtained from Different Sources by HPLC/DAD. Journal of Analytical Methods in Chemistry, 2014, 2014, 1-5.	0.7	23
58	Experimental designs characterizing seasonal variations and solvent effects on the quantities of coumarin and related metabolites from Mikania laevigata. Analytica Chimica Acta, 2014, 821, 89-96.	2.6	18
59	Open column, reversed-phase high-performance liquid chromatography with diode array detection and chemometric strategy for investigation of metabolic fingerprints of complex systems. Analytical Methods, 2014, 6, 9567-9574.	1.3	3
60	An atom in molecules study of infrared intensity enhancements in fundamental donor stretching bands in hydrogen bond formation. Physical Chemistry Chemical Physics, 2014, 16, 24920-24928.	1.3	13
61	Atomic charge transfer-counter polarization effects determine infrared CH intensities of hydrocarbons: a quantum theory of atoms in molecules model. Physical Chemistry Chemical Physics, 2014, 16, 23224-23232.	1.3	16
62	Coreâ€“valence correlation effects on IR calculations: the BF3 and BCl3 cases. Journal of Molecular Modeling, 2014, 20, 2333.	0.8	2
63	Quantum Theory of Atoms in Molecules/Chargeâ€“Charge Fluxâ€“Dipole Flux interpretation of fundamental vibrational intensity enhancements on H-bond formation of water trimer. Chemical Physics Letters, 2014, 610-611, 14-18.	1.2	9
64	Quantum theory of atoms in molecules/charge-charge flux-dipole flux models for fundamental vibrational intensity changes on H-bond formation of water and hydrogen fluoride. Journal of Chemical Physics, 2014, 140, 084306.	1.2	11
65	Doehlert design-desirability function multi-criteria optimal separation of 17 phenolic compounds from extra-virgin olive oil by capillary zone electrophoresis. Food Chemistry, 2014, 146, 558-568.	4.2	27
66	QTAIM chargeâ€“charge fluxâ€“dipole flux models for the fundamental infrared intensities of BF3 and BCl3. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 116, 136-142.	2.0	6
67	Optimization of Electrophoretic Separations of Thirteen Phenolic Compounds using Single Peak Responses and an Interactive Computer Technique. Journal of the Brazilian Chemical Society, 2013, , .	0.6	1
68	How Accessible Is Atomic Charge Information from Infrared Intensities? A QTAIM/CCFDF Interpretation. Journal of Physical Chemistry A, 2012, 116, 8238-8249.	1.1	40
69	Principal component and Tucker3 analyses of high performance liquid chromatography with diode-array detection fingerprints of crude extracts of Erythrina speciosa Andrews leaves. Analytica Chimica Acta, 2012, 736, 36-44.	2.6	13
70	Development of a new topological index for the prediction of normal boiling point temperatures of hydrocarbons: The Fi index. Journal of Molecular Liquids, 2012, 165, 125-132.	2.3	18
71	Basis set selection for the calculation of the IR fundamental intensities for 1,1-C2H2F2 and F2CO. Journal of Molecular Structure, 2012, 1009, 49-54.	1.8	5
72	QTAIM Chargeâ€“Charge Fluxâ€“Dipole Flux Interpretation of Electronegativity and Potential Models of the Fluorochloromethane Mean Dipole Moment Derivatives. Journal of Physical Chemistry A, 2011, 115, 12572-12581.	1.1	8

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73	Mixture designs for exploring class diversity and metabolite fingerprinting: An efficient column chromatographic strategy. Analytica Chimica Acta, 2011, 702, 288-294.	2.6	11
74	Use of multivariate statistical techniques to optimize the simultaneous separation of 13 phenolic compounds from extra-virgin olive oil by capillary electrophoresis. Talanta, 2011, 83, 1181-1187.	2.9	52
75	Chemometrics optimization of carbohydrate separations in six food matrices by micellar electrokinetic chromatography with anionic surfactant. Talanta, 2011, 85, 237-244.	2.9	17
76	EstatÃstica aplicada Ã quÃmica: dez dÃºvidas comuns. Quimica Nova, 2011, 34, 888-892.	0.3	9
77	Mixture Design Optimization of an Analytical Procedure for Iron Extraction and Determination From Cassava Leaves by Slurry Sampling Flame Atomic Absorption Spectrometry. Spectroscopy Letters, 2011, 44, 388-392.	0.5	9
78	Comparison of Emission of Dioxins and Furans from Gasohol- and Ethanol-Powered Vehicles. Journal of the Air and Waste Management Association, 2011, 61, 1344-1352.	0.9	3
79	Mixture Design and Response Surface Analysis of Densification of Silicon Carbide Ceramics with (SiO₂â€“Dy₂O₃â€“Al₂O₃) Additives. International Journal of Applied Ceramic Technology, 2010, 7, 493-501.	1.1	3
80	Factorial design to optimize microwave-assisted synthesis of FDU-1 silica with a new triblock copolymer. Microporous and Mesoporous Materials, 2010, 133, 1-9.	2.2	11
81	Optimisation of a CE method for caffeine analysis in decaffeinated coffee. Food Chemistry, 2010, 120, 1155-1161.	4.2	47
82	Principal component analysis and hierarchical cluster analysis for homogeneity evaluation during the preparation of a wheat flour laboratory reference material for inorganic analysis. Microchemical Journal, 2010, 95, 222-226.	2.3	40
83	Statistical mixture design â€” Principal component determination of synergic solvent interactions for natural product extractions. Chemometrics and Intelligent Laboratory Systems, 2010, 103, 1-7.	1.8	26
84	Coupled cluster and configuration interaction quantum calculations of infrared fundamental intensities. International Journal of Quantum Chemistry, 2010, 110, 2029-2036.	1.0	4
85	STATISTICAL DESIGN OF EXPERIMENTS FOR OPTIMIZATION OF BATCH ADSORPTION CONDITIONS FOR REMOVAL OF REACTIVE RED 194 TEXTILE DYE FROM AQUEOUS EFFLUENTS. Chemical Engineering Communications, 2010, 197, 775-790.	1.5	20
86	Synthesis Optimization of Hydroxymethylnitrofurazone, an Antichagasic Candidate, Using 32 Factorial Design. Letters in Organic Chemistry, 2010, 7, 191-195.	0.2	5
87	Simultaneous determination of first-line anti-tuberculosis drugs by capillary zone electrophoresis using direct UV detection. Talanta, 2010, 82, 333-339.	2.9	45
88	Multivariate optimization and validation of an analytical method for the determination of cadmium in wines employing ET AAS. Journal of the Brazilian Chemical Society, 2009, 20, 788-794.	0.6	12
89	Emission of polycyclic aromatic hydrocarbons from gasohol and ethanol vehicles. Atmospheric Environment, 2009, 43, 648-654.	1.9	54
90	Statistical mixture design investigation of fractionated and total extracts from Erythrina speciosa Andrews leaves. Journal of Separation Science, 2009, 32, 644-652.	1.3	25

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91	Combined columnâ€“mobile phase mixture statistical design optimization of high-performance liquid chromatographic analysis of multicomponent systems. Journal of Chromatography A, 2009, 1216, 1439-1449.	1.8	25
92	Factorial design preparation of transparent conducting oxide thin films. Thin Solid Films, 2009, 517, 2886-2891.	0.8	7
93	Quantum Theory Atoms in Molecules Chargeâ^'Charge Fluxâ^'Dipole Flux Models for the Infrared Intensities of Benzene and Hexafluorobenzene. Journal of Physical Chemistry A, 2009, 113, 7972-7978.	1.1	5
94	Statistical mixture design development of digestion methods for Oyster tissue using inductively coupled plasma optical emission spectrometry for the determination of metallic ions. Talanta, 2009, 80, 559-564.	2.9	17
95	Statistical mixture designâ€"Varimax factor optimization for selective compound extraction from plant material. Analytica Chimica Acta, 2008, 613, 48-55.	2.6	19
96	ChelpG and QTAIM atomic charge and dipole models for the infrared fundamental intensities of the fluorochloromethanes. Theoretical Chemistry Accounts, 2008, 121, 173-179.	0.5	22
97	The removal of the indigo carmine dye from aqueous solutions using cross-linked chitosanâ€"Evaluation of adsorption thermodynamics using a full factorial design. Journal of Hazardous Materials, 2008, 153, 566-574.	6.5	97
98	Optimization of an electrolyte system for analysis of ethambutol in pharmaceutical formulations by capillary zone electrophoresis using complexation with copper(II). Journal of Chromatography A, 2008, 1202, 224-228.	1.8	20
99	A Glimpse of Recent Developments in Brazilian Analytical Chemistry. Analytical Letters, 2008, 41, 1494-1546.	1.0	1
100	Determination of Cd, Cu, and Pb after Cloud Point Extraction using Multielemental Sequential Determination by Thermospray Flame Furnace Atomic Absorption Spectrometry (TSâ€FFâ€AAS). Separation Science and Technology, 2008, 43, 815-827.	1.3	25
101	Eucalyptus Tar Pitch Substitution of Phenol in the Preparation of Novolak-Type Resins Cured with Hexamethylenetetramine. Bulletin of the Chemical Society of Japan, 2008, 81, 1528-1533.	2.0	1
102	ImplementaÃ§Ã£o computacional do modelo carga-fluxo de carga-fluxo de dipolo para cÃ¡lculo e interpretaÃ§Ã£o das intensidades do espectro infravermelho. Quimica Nova, 2008, 31, 1750-1754.	0.3	18
103	Mineral composition of wheat flour consumed in Brazilian cities. Journal of the Brazilian Chemical Society, 2008, 19, 935-942.	0.6	36
104	Technological aspects for restructuring concentrated pineapple pulp. LWT - Food Science and Technology, 2007, 40, 759-765.	2.5	8
105	Quantum Theory of Atoms in Molecules Chargeâ^'Charge Fluxâ^'Dipole Flux Models for the Infrared Intensities of X₂CY (X = H, F, Cl; Y = O, S) Molecules. Journal of Physical Chemistry A, 2007, 111, 7870-7875.	1.1	22
106	QTAIM Chargeâ^'Charge Fluxâ^'Dipole Flux Models for the Infrared Fundamental Intensities of Difluoro- and Dichloroethylenes. Journal of Physical Chemistry A, 2007, 111, 515-520.	1.1	17
107	Statistical mixture design â€" principal component optimization for selective compound extraction from plant material. Journal of Separation Science, 2007, 30, 3302-3310.	1.3	12
108	Study of the reaction conditions for the hydrodechlorination of pentachlorophenol on palladium catalysts. Chemical Engineering Journal, 2007, 131, 59-64.	6.6	13

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109	Unreplicated split-plot mixture designs and statistical models for optimizing mobile chromatographic phase and extraction solutions for fingerprint searches. Chemometrics and Intelligent Laboratory Systems, 2007, 89, 82-89.	1.8	8
110	Statistical designs and response surface techniques for the optimization of chromatographic systems. Journal of Chromatography A, 2007, 1158, 2-14.	1.8	493
111	Mixtureâ€“mixture design for the fingerprint optimization of chromatographic mobile phases and extraction solutions for Camellia sinensis. Analytica Chimica Acta, 2007, 595, 28-37.	2.6	30
112	Box-Behnken design: An alternative for the optimization of analytical methods. Analytica Chimica Acta, 2007, 597, 179-186.	2.6	2,226
113	Automatic on-line pre-concentration system using a knotted reactor for the FAAS determination of lead in drinking water. Journal of Hazardous Materials, 2007, 141, 540-545.	6.5	23
114	The removal of Cu(II) and Co(II) from aqueous solutions using cross-linked chitosanâ€”Evaluation by the factorial design methodology. Journal of Hazardous Materials, 2007, 143, 8-16.	6.5	45
115	Water-Soluble Ions and Trace Metals in Airborne Particles Over Urban Areas of the State of SÃ£o Paulo, Brazil: Influences of Local Sources and Long Range Transport. Water, Air, and Soil Pollution, 2007, 186, 63-73.	1.1	35
116	Hidrocarbonetos policÃclicos aromÃ¡ticos como traÃ§adores da queima de cana-de-aÃ§Ãºcar: uma abordagem estatÃstica. Quimica Nova, 2007, 30, 577-581.	0.3	29
117	ConseqÃ¼Ãªncias da anÃ¡lise incorreta de experimentos blocados. Quimica Nova, 2007, 30, 436-440.	0.3	0
118	PrecisÃ£o dos mÃ©todos refratomÃ©tricos para anÃ¡lise de umidade em mel. Food Science and Technology, 2007, 27, 328-332.	0.8	0
119	QTAIM Chargeâ€'Charge Fluxâ€'Dipole Flux Models for the Infrared Fundamental Intensities of the Fluorochloromethanes. Journal of Physical Chemistry A, 2006, 110, 4839-4845.	1.1	26
120	Optimization of mobile phase for separation of carbohydrates in honey by high performance liquid chromatography using a mixture design. Journal of the Brazilian Chemical Society, 2006, 17, 588-593.	0.6	9
121	25 anos de quimiometria no Brasil. Quimica Nova, 2006, 29, 1401-1406.	0.3	22
122	Electrospray ionization mass spectrometry fingerprinting of perfumes: rapid classification and counterfeit detection. Rapid Communications in Mass Spectrometry, 2006, 20, 3654-3658.	0.7	21
123	Factorial design optimization of solid phase microextraction conditons for gas chromatographyâ€“mass spectrometry (GCâ€“MS) analysis of linear alkylbenzenes (LABs) in detergents. Analytica Chimica Acta, 2006, 562, 152-157.	2.6	19
124	Statistical design-principal component analysis optimization of a multiple response procedure using cloud point extraction and simultaneous determination of metals by ICP OES. Analytica Chimica Acta, 2006, 580, 251-257.	2.6	66
125	Chapter 3 Changing everything at the same time. Data Handling in Science and Technology, 2005, 25, 83-145.	3.1	2
126	Chapter 2 When the situation is normal. Data Handling in Science and Technology, 2005, 25, 9-81.	3.1	1

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127	32 Factorial design and response surface analysis optimization of N-carboxybutylchitosan synthesis. Carbohydrate Polymers, 2005, 59, 37-42.	5.1	30
128	Split-plot designs and normal probability graphs for the optimization of chemical systems. Analytica Chimica Acta, 2005, 544, 206-212.	2.6	7
129	A chargeâ€“charge fluxâ€“dipole flux decomposition of the dipole moment derivatives and infrared intensities of the AB3 (A=N, P; B=H, F) molecules. Chemical Physics, 2005, 317, 35-42.	0.9	20
130	Chapter 6 Exploring the response surface. Data Handling in Science and Technology, 2005, 25, 245-312.	3.1	4
131	An Atomic Chargeâ^'Charge Fluxâ^'Dipole Flux Atom-in-Molecule Decomposition for Molecular Dipole-Moment Derivatives and Infrared Fundamental Intensities. Journal of Physical Chemistry A, 2005, 109, 2680-2688.	1.1	80
132	Dioxins and furans in the atmosphere of SÃ£o Paulo City, Brazil. Chemosphere, 2005, 58, 1391-1398.	4.2	35
133	InfluÃªncia do material e volume do porta-amostra na determinaÃ§Ã£o termogravimÃ©trica do teor de cinzas em mel. Quimica Nova, 2005, 28, 713-715.	0.3	2
134	OtimizaÃ§Ã£o via metodologia de superfÃcie de respostas dos parÃ¢metros tecnolÃ³gicos para produÃ§Ã£o de fruta estruturada e desidratada a partir de polpa concentrada de mamÃ£o. Food Science and Technology, 2005, 25, 158-164.	0.8	9
135	Reducing the number of experiments in split-plot optimization designs. Journal of the Brazilian Chemical Society, 2004, 15, 241-245.	0.6	1
136	Application of steady-state and dynamic modeling for the prediction of the BOD of an aerated lagoon at a pulp and paper mill. Chemical Engineering Journal, 2004, 104, 73-81.	6.6	23
137	Application of steady-state and dynamic modeling for the prediction of the BOD of an aerated lagoon at a pulp and paper millPart II. Nonlinear approaches. Chemical Engineering Journal, 2004, 105, 61-69.	6.6	40
138	Characterization of monofloral honeys by ash contents through a hierarchical design. Journal of Food Composition and Analysis, 2004, 17, 737-747.	1.9	27
139	The infrared vibrational intensities and polar tensors of HFCO and DFCO. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 2947-2952.	2.0	8
140	Full factorial design applied to intercalation of amines in lamellar titanium phenylphosphonate and titanium phenylarsonate. Journal of Solid State Chemistry, 2004, 177, 675-680.	1.4	8
141	Split-plot design optimization for trace determination of lead by anodic stripping voltammetry in a homogeneous ternary solvent system. Chemometrics and Intelligent Laboratory Systems, 2004, 70, 113-121.	1.8	11
142	An application of chemometric techniques to analyze the effects of the wave function modifications on the intermolecular stretching frequencies of the hydrogen-bonded complexes. Chemometrics and Intelligent Laboratory Systems, 2004, 70, 157-163.	1.8	6
143	Characteristic Substituent-Shift Models for Carbon 1s Ionization Energies and Mean Dipole-Moment Derivatives. Journal of Physical Chemistry A, 2004, 108, 866-873.	1.1	11
144	Atomic Mean Dipole Moment Derivative and Anisotropic Contributions to Molecular Infrared Intensity Sums. Journal of Physical Chemistry A, 2004, 108, 6788-6796.	1.1	12

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145	Evaluation of the salt accumulation process during inundation in water resource of Contas river basin (Bahiaâ€“Brazil) applying principal component analysis. Water Research, 2004, 38, 1579-1585.	5.3	25
146	Optimization of thermogravimetric analysis of ash content in honey. Journal of the Brazilian Chemical Society, 2004, 15, 797-802.	0.6	18
147	Simulation of Aerated Lagoon Using Artificial Neural Networks and Multivariate Regression Techniques. Applied Biochemistry and Biotechnology, 2003, 106, 437-450.	1.4	3
148	Title is missing!. Journal of Applied Electrochemistry, 2003, 33, 1069-1075.	1.5	14
149	The infrared fundamental intensities and polar tensor of CH3NC. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 37-45.	2.0	1
150	Artifact evidence in carbonyl compound sampling using the enclosure technique with cuvette system. Journal of Environmental Monitoring, 2003, 5, 795.	2.1	3
151	Core Ionization Energies, Mean Dipole Moment Derivatives, and Simple Potential Models for B, N, O, F, P, Cl, and Br Atoms in Molecules. Journal of Physical Chemistry A, 2002, 106, 1824-1833.	1.1	6
152	The linear relationship between Koopmans' and hydrogen bond energies for some simple carbonyl molecules. Journal of the Brazilian Chemical Society, 2002, 13, 800.	0.6	7
153	Simulation of an industrial wastewater treatment plant using artificial neural networks and principal components analysis. Brazilian Journal of Chemical Engineering, 2002, 19, 365-370.	0.7	68
154	Methylene blue immobilized on cellulose surfaces modified with titanium dioxide and titanium phosphate: factorial design optimization of redox properties. Journal of Electroanalytical Chemistry, 2002, 531, 141-146.	1.9	25
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