Guillermo QuintÃs

List of Publications by Year
in descending order

124 papers	2,973 citations	172457 29 h-index	243625 44 g-index
128 all docs	128 docs citations	128 times ranked	4269 citing authors

#	Article	IF	Citations
1	Dichloro-dihydro-fluorescein diacetate (DCFH-DA) assay: A quantitative method for oxidative stress assessment of nanoparticle-treated cells. Toxicology in Vitro, 2013, 27, 954-963.	2.4	349
2	Intra-batch effect correction in liquid chromatography-mass spectrometry using quality control samples and support vector regression (QC-SVRC). Analyst, The, 2015, 140, 7810-7817.	3.5	96
3	Determination of Peroxide-Based Explosives Using Liquid Chromatography with On-Line Infrared Detection. Analytical Chemistry, 2006, 78, 8150-8155.	6.5	82
4	Determination of PAHs in airborne particles by accelerated solvent extraction and large-volume injection–gas chromatography–mass spectrometry. Talanta, 2006, 69, 807-815.	5.5	63
5	Plasma sample based analysis of gastric cancer progression using targeted metabolomics. Scientific Reports, 2017, 7, 17774.	3.3	56
6	Chemometric approaches to improve PLSDA model outcome for predicting human non-alcoholic fatty liver disease using UPLC-MS as a metabolic profiling tool. Metabolomics, 2012, 8, 86-98.	3.0	54
7	Bladder cancer recurrence surveillance by urine metabolomics analysis. Scientific Reports, 2018, 8, 9172.	3.3	54
8	Urinary Lipid Peroxidation Byproducts: Are They Relevant for Predicting Neonatal Morbidity in Preterm Infants?. Antioxidants and Redox Signaling, 2015, 23, 178-184.	5.4	53
9	Non-invasive prediction of NAFLD severity: a comprehensive, independent validation of previously postulated serum microRNA biomarkers. Scientific Reports, 2018, 8, 10606.	3.3	52
10	Mid-infrared and Raman spectrometry for quality control of pesticide formulations. TrAC - Trends in Analytical Chemistry, 2005, 24, 772-781.	11.4	51
11	Determination of acrylamide in foods by pressurized fluid extraction and liquid chromatography-tandem mass spectrometry used for a survey of Spanish cereal-based foods. Food Additives and Contaminants, 2006, 23, 237-244.	2.0	44
12	Evaluation of batch effect elimination using quality control replicates in LC-MS metabolite profiling. Analytica Chimica Acta, 2018, 1019, 38-48.	5.4	42
13	Automated sample preparation and analysis using a sequential-injection–capillary electrophoresis (SI–CE) interface. Analyst, The, 2006, 131, 739-744.	3.5	40
14	Analysis of lipid peroxidation biomarkers in extremely low gestational age neonate urines by UPLC-MS/MS. Analytical and Bioanalytical Chemistry, 2014, 406, 4345-4356.	3.7	40
15	On-Capillary Surface-Enhanced Raman Spectroscopy: Determination of Glutathione in Whole Blood Microsamples. Analytical Chemistry, 2018, 90, 9093-9100.	6.5	40
16	A validated and fast procedure for FTIR determination of Cypermethrin and Chlorpyrifos. Talanta, 2005, 67, 634-639.	5.5	39
17	Analytical potential of mid-infrared detection in capillary electrophoresis and liquid chromatography: A review. Analytica Chimica Acta, 2010, 679, 31-42.	5.4	39
18	Background Correction and Multivariate Curve Resolution of Online Liquid Chromatography with Infrared Spectrometric Detection. Analytical Chemistry, 2011, 83, 4855-4862.	6.5	39

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19	Predicting survival of patients with hypocellular myelodysplastic syndrome. Cancer, 2012, 118, 4462-4470.	4.1	38
20	On-line gel permeation chromatography–attenuated total reflectance–Fourier transform infrared determination of lecithin and soybean oil in dietary supplements. Journal of Chromatography A, 2008, 1185, 71-77.	3.7	35
21	A rapid method for the differentiation of yeast cells grown under carbon and nitrogen-limited conditions by means of partial least squares discriminant analysis employing infrared micro-spectroscopic data of entire yeast cells. Talanta, 2012, 99, 566-573.	5.5	35
22	Simultaneous determination of Folpet and Metalaxyl in pesticide formulations by flow injection Fourier transform infrared spectrometry. Analytica Chimica Acta, 2003, 480, 11-21.	5.4	34
23	Direct determination of polymerised triacylglycerides in deep-frying vegetable oil by near infrared spectroscopy using Partial Least Squares regression. Food Chemistry, 2012, 131, 353-359.	8.2	33
24	Metabolomic Analysis of Gastric Cancer Progression within the Correa's Cascade Using Ultraperformance Liquid Chromatography–Mass Spectrometry. Journal of Proteome Research, 2016, 15, 2729-2738.	3.7	32
25	Model selection for within-batch effect correction in UPLC-MS metabolomics using quality control - Support vector regression. Analytica Chimica Acta, 2018, 1026, 62-68.	5.4	32
26	New cut-off criterion for uninformative variable elimination in multivariate calibration of near-infrared spectra for the determination of heroin in illicit street drugs. Analytica Chimica Acta, 2008, 630, 150-160.	5.4	31
27	Determination of lecithin and soybean oil in dietary supplements using partial least squares–Fourier transform infrared spectroscopy. Talanta, 2008, 77, 229-234.	5.5	31
28	The value of selected in vitro and in silico methods to predict acute oral toxicity in a regulatory context: Results from the European Project ACuteTox. Toxicology in Vitro, 2013, 27, 1357-1376.	2.4	31
29	Integrative Metabolomic and Transcriptomic Analysis for the Study of Bladder Cancer. Cancers, 2019, 11, 686.	3.7	31
30	FT–Raman spectrometry determination of Malathion in pesticide formulations. Talanta, 2004, 63, 345-350.	5.5	30
31	Modified locally weighted–Partial least squares regression improving clinical predictions from infrared spectra of human serum samples. Talanta, 2013, 107, 368-375.	5.5	30
32	Novel free-radical mediated lipid peroxidation biomarkers in newborn plasma. Analytica Chimica Acta, 2017, 996, 88-97.	5.4	30
33	Fourier transform infrared spectrometric strategies for the determination of Buprofezin in pesticide formulations. Analytica Chimica Acta, 2002, 468, 81-90.	5.4	29
34	Comparing Targeted vs. Untargeted MS2 Data-Dependent Acquisition for Peak Annotation in LC–MS Metabolomics. Metabolites, 2020, 10, 126.	2.9	29
35	Determination of caffeine in tea samples by Fourier transform infrared spectrometry. Analytical and Bioanalytical Chemistry, 2002, 374, 561-565.	3.7	28
36	Assessment of Oxidative Damage to Proteins and DNA in Urine of Newborn Infants by a Validated UPLC-MS/MS Approach. PLoS ONE, 2014, 9, e93703.	2.5	28

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37	Recent advances in on-line liquid chromatography - infrared spectrometry (LC-IR). TrAC - Trends in Analytical Chemistry, 2010, 29, 544-552.	11.4	27
38	Detection of batch effects in liquid chromatography-mass spectrometry metabolomic data using guided principal component analysis. Talanta, 2014, 130, 442-448.	5.5	27
39	Fourier transform infrared determination of imidacloprid in pesticide formulations. Journal of the Brazilian Chemical Society, 2004, 15, 307-312.	0.6	26
40	New background correction approach based on polynomial regressions for on-line liquid chromatographyâ€"Fourier transform infrared spectrometry. Journal of Chromatography A, 2009, 1216, 3122-3130.	3.7	26
41	Monitoring of system conditioning after blank injections in untargeted UPLC-MS metabolomic analysis. Scientific Reports, 2019, 9, 9822.	3.3	26
42	Immunosuppressive profiles in liquid biopsy at diagnosis predict response to neoadjuvant chemotherapy in triple-negative breast cancer. European Journal of Cancer, 2020, 139, 119-134.	2.8	26
43	Fourier transform infrared spectrometric determination of Malathion in pesticide formulations. Analytica Chimica Acta, 2004, 502, 213-220.	5.4	25
44	Determination of cyromazine in pesticide commercial formulations by vibrational spectrometric procedures. Analytica Chimica Acta, 2004, 524, 257-264.	5.4	25
45	Univariate method for background correction in liquid chromatographyâ€"Fourier transform infrared spectrometry. Journal of Chromatography A, 2008, 1190, 102-109.	3.7	25
46	Plasma metabolite score correlates with Hypoxia time in a newly born piglet model for asphyxia. Redox Biology, 2017, 12, 1-7.	9.0	25
47	On-Line Fourier Transform Infrared Spectrometric Detection in Gradient Capillary Liquid Chromatography Using Nanoliter-Flow Cells. Analytical Chemistry, 2009, 81, 3746-3753.	6.5	24
48	High performance liquid chromatography with mid-infrared detection based on a broadly tunable quantum cascade laser. Analyst, The, 2014, 139, 2057.	3.5	24
49	Changes of the plasma metabolome of newly born piglets subjected to postnatal hypoxia and resuscitation with air. Pediatric Research, 2016, 80, 284-292.	2.3	24
50	Surface enhanced Raman spectroscopic direct determination of low molecular weight biothiols in umbilical cord whole blood. Analyst, The, 2016, 141, 2165-2174.	3.5	24
51	Metabolomic analysis to discriminate drug-induced liver injury (DILI) phenotypes. Archives of Toxicology, 2021, 95, 3049-3062.	4.2	24
52	High performance liquid chromatography with on-line dual quantum cascade laser detection for the determination ofÂcarbohydrates, alcohols and organic acids in wine and grape juice. Applied Physics B: Lasers and Optics, 2010, 99, 833-840.	2.2	23
53	Effect of donor human milk on host-gut microbiota and metabolic interactions in preterm infants. Clinical Nutrition, 2021, 40, 1296-1309.	5.0	23
54	External cavity-quantum cascade laser (EC-QCL) spectroscopy for protein analysis in bovine milk. Analytica Chimica Acta, 2017, 963, 99-105.	5.4	22

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55	Evaluation of the effect of chance correlations on variable selection using Partial Least Squares-Discriminant Analysis. Talanta, 2013, 116, 835-840.	5.5	21
56	Analysis of multi-source metabolomic data using joint and individual variation explained (JIVE). Analyst, The, 2015, 140, 4521-4529.	3.5	21
57	Current Practice in Untargeted Human Milk Metabolomics. Metabolites, 2020, 10, 43.	2.9	21
58	On-line gradient liquid chromatographyâ€"Fourier transform infrared spectrometry determination of sugars in beverages using chemometric background correction. Talanta, 2008, 77, 779-785.	5.5	20
59	Sample classification for improved performance of PLS models applied to the quality control of deep-frying oils of different botanic origins analyzed using ATR-FTIR spectroscopy. Analytical and Bioanalytical Chemistry, 2011, 399, 1305-1314.	3.7	19
60	Assessment of the statistical significance of classifications in infrared spectroscopy based diagnostic models. Analyst, The, 2015, 140, 2422-2427.	3.5	19
61	Fast quantification of bovine milk proteins employing external cavity-quantum cascade laser spectroscopy. Food Chemistry, 2018, 252, 22-27.	8.2	19
62	Urinary Metabolic Signatures Detect Recurrences in Non-Muscle Invasive Bladder Cancer. Cancers, 2019, 11, 914.	3.7	19
63	Urine metabolomic analysis for monitoring internal load in professional football players. Metabolomics, 2020, 16, 45.	3.0	19
64	Metabolomic Analysis of the Effect of Postnatal Hypoxia on the Retina in a Newly Born Piglet Model. PLoS ONE, 2013, 8, e66540.	2.5	19
65	Detection of prostate cancer using a voltammetric electronic tongue. Analyst, The, 2016, 141, 4562-4567.	3.5	18
66	High and ultraâ€high definition of infrared spectral histopathology gives an insight into chemical environment of lung metastases in breast cancer. Journal of Biophotonics, 2019, 12, e201800345.	2.3	18
67	FTIR Approaches for Diuron Determination in Commercial Pesticide Formulations. Journal of Agricultural and Food Chemistry, 2005, 53, 5842-5847.	5.2	17
68	Determination of critical eluent composition for polyethylenglycols using on-line liquid chromatographyâ€"Fourier transform infrared spectrometry. Analytica Chimica Acta, 2008, 624, 278-285.	5.4	17
69	Assessment of discriminant models in infrared imaging using constrained repeated random sampling â€" Cross validation. Analytica Chimica Acta, 2018, 1033, 156-164.	5.4	17
70	Direct determination of polymerized triglycerides in deep-frying olive oil by attenuated total reflectanceâ€"Fourier transform infrared spectroscopy using partial least squares regression. Analytical and Bioanalytical Chemistry, 2010, 397, 861-869.	3.7	16
71	Assessment of phospholipid synthesis related biomarkers for perinatal asphyxia: a piglet study. Scientific Reports, 2017, 7, 40315.	3.3	16
72	The Potential Role of Metabolomics in Drug-Induced Liver Injury (DILI) Assessment. Metabolites, 2022, 12, 564.	2.9	16

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73	Fourier transform infrared determination of Fluometuron in pesticide formulations. Vibrational Spectroscopy, 2003, 31, 63-69.	2.2	15
74	Application of point-to-point matching algorithms for background correction in on-line liquid chromatographyâ€"Fourier transform infrared spectrometry (LCâ€"FTIR). Talanta, 2010, 80, 1771-1776.	5.5	15
75	Towards the potential use of ^{1}H NMR spectroscopy in urine samples for prostate cancer detection. Analyst, The, 2014, 139, 3875-3878.	3.5	15
76	Monitoring of Polymerized Triglycerides in Deep-Frying Oil by On-Line GPC-FTIR Spectrometry Using the Science Based Calibration Multivariate Approach. Chromatographia, 2010, 71, 201-209.	1.3	14
77	Metabolic Phenotypes of Hypoxic-Ischemic Encephalopathy with Normal vs. Pathologic Magnetic Resonance Imaging Outcomes. Metabolites, 2020, 10, 109.	2.9	14
78	Application of Discriminant Analysis and Cross-Validation on Proteomics Data. Methods in Molecular Biology, 2016, 1362, 175-184.	0.9	14
79	Chemometric extraction of analyteâ€specific chromatograms in onâ€line gradient LCâ€infrared spectrometry. Journal of Separation Science, 2009, 32, 4089-4095.	2.5	13
80	Troubleshooting in Large-Scale LC-ToF-MS Metabolomics Analysis: Solving Complex Issues in Big Cohorts. Metabolites, 2019, 9, 247.	2.9	13
81	Discriminant analysis and feature selection in mass spectrometry imaging using constrained repeated random sampling - Cross validation (CORRS-CV). Analytica Chimica Acta, 2020, 1097, 30-36.	5.4	13
82	Analysis of the Association between Fatigue and the Plasma Lipidomic Profile of Inflammatory Bowel Disease Patients. Journal of Proteome Research, 2021, 20, 381-392.	3.7	13
83	FT-Raman determination of Mepiquat chloride in agrochemical products. Vibrational Spectroscopy, 2004, 36, 41-46.	2.2	12
84	Determination of glycolic acid in cosmetics by online liquid chromatographyâ€"Fourier transform infrared spectrometry. Analytical and Bioanalytical Chemistry, 2008, 392, 1383-1389.	3.7	12
85	Cubic smoothing splines background correction in on-line liquid chromatographyâ€"Fourier transform infrared spectrometry. Journal of Chromatography A, 2010, 1217, 6733-6741.	3.7	12
86	Metabolic adaptation and neuroprotection differ in the retina and choroid in a piglet model of acute postnatal hypoxia. Pediatric Research, 2014, 76, 127-134.	2.3	12
87	Atmospheric Compensation in Fourier Transform Infrared (FT-IR) Spectra of Clinical Samples. Applied Spectroscopy, 2013, 67, 1339-1342.	2.2	11
88	ATR-FTIR spectroscopy for the routine quality control of exosome isolations. Chemometrics and Intelligent Laboratory Systems, 2021, 217, 104401.	3.5	11
89	Development of a simple and low cost device for vapour phase Fourier Transform Infrared spectrometry determination of ethanol in mouthwashes. Analytica Chimica Acta, 2006, 569, 238-243.	5.4	10
90	Determination of enzyme activity inhibition by FTIR spectroscopy on the example of fructose bisphosphatase. Analytical and Bioanalytical Chemistry, 2009, 394, 2137-2144.	3.7	10

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91	Prolonging in utero-like oxygenation after birth diminishes oxidative stress in the lung and brain of mice pups. Redox Biology, 2013, 1, 297-303.	9.0	10
92	Improving the performance of hollow waveguide-based infrared gas sensors via tailored chemometrics. Analytical and Bioanalytical Chemistry, 2013, 405, 8223-8232.	3.7	10
93	Adrenic acid non-enzymatic peroxidation products in biofluids of moderate preterm infants. Free Radical Biology and Medicine, 2019, 142, 107-112.	2.9	10
94	Data mining Raman microspectroscopic responses of cells to drugs in vitro using multivariate curve resolution-alternating least squares. Talanta, 2020, 208, 120386.	5.5	10
95	Infrared biospectroscopy for a fast qualitative evaluation of sample preparation in metabolomics. Talanta, 2014, 127, 181-190.	5.5	9
96	Noninvasive monitoring of evolving urinary metabolic patterns in neonatal encephalopathy. Pediatric Research, 2022, 91, 598-605.	2.3	9
97	Factors that influence the quality of metabolomics data in in vitro cell toxicity studies: a systematic survey. Scientific Reports, 2021, 11, 22119.	3.3	9
98	First‐Derivative Fourier‐Transform Infrared Determination of Oxadiazon in Commercial Herbicide Formulations. Spectroscopy Letters, 2008, 41, 1-8.	1.0	8
99	Toward Rapid Screening of Liver Grafts at the Operating Room Using Mid-infrared Spectroscopy. Analytical Chemistry, 2020, 92, 14542-14549.	6.5	8
100	The effect of Holder pasteurization on the lipid and metabolite composition of human milk. Food Chemistry, 2022, 384, 132581.	8.2	8
101	Procedure for Automated Background Correction in Flow Systems with Infrared Spectroscopic Detection and Changing Liquid-Phase Composition. Applied Spectroscopy, 2009, 63, 1363-1369.	2.2	7
102	On-line capillary electrophoresis FTIR detection for the separation and characterization of proteins. Vibrational Spectroscopy, 2006, 42, 392-396.	2.2	6
103	On-line monitoring of pH junctions in capillary electrophoresis using Fourier transform infrared spectrometry. Analytical and Bioanalytical Chemistry, 2006, 387, 287-292.	3.7	6
104	First-order derivative resolution of overlapped PAH peaks with common mass spectra in gas chromatography–mass spectrometry. Talanta, 2008, 74, 747-752.	5.5	6
105	HPLC determination of oxadiazon in commercial pesticide formulations. Journal of the Brazilian Chemical Society, 2008, 19, 1394-1398.	0.6	6
106	Data Quality Assessment in Untargeted LC-MS Metabolomics. Comprehensive Analytical Chemistry, 2018, 82, 137-164.	1.3	6
107	Extracting consistent biological information from functional results of metabolomic pathway analysis using the Mantel's test. Analytica Chimica Acta, 2021, 1187, 339173.	5.4	6
108	Science based calibration for the extraction of 'analyte-specific' HPLC-DAD chromatograms in environmental analysis. Talanta, 2011, 83, 1158-1165.	5.5	5

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109	Metabolomic profiling in neuroblastoma. Pediatric Blood and Cancer, 2020, 67, e28113.	1.5	5
110	Direct Derivatization in Dried Blood Spots for Oxidized and Reduced Glutathione Quantification in Newborns. Antioxidants, 2022, 11, 1165.	5.1	4
111	Advanced IR and Raman detectors for identification and quantification. , 2017, , 463-477.		3
112	A Novel UPLC-MS Metabolomic Analysis-Based Strategy to Monitor the Course and Extent of iPSC Differentiation to Hepatocytes. Journal of Proteome Research, 2022, , .	3.7	3
113	An Infrared Method, with Reduced Solvent Consumption, for the Determination of Chlorsulfuron in Pesticide Formulations. Spectroscopy Letters, 2003, 36, 515-529.	1.0	2
114	Towards minimization of chlorinated solvents consume in Fourier transform infrared spectroscopy determination of Propamocarb in pesticide formulations. Talanta, 2008, 75, 339-343.	5.5	2
115	Liquid Chromatographyâ€"Liquid Chromatographyâ€"Fourier Transform Infrared. , 2018, , 75-75.		2
116	A Reductive Metabolic Switch Protects Infants with Transposition of Great Arteries Undergoing Atrial Septostomy against Oxidative Stress. Antioxidants, 2021, 10, 1502.	5.1	2
117	Determination of pirimicarb and endosulfan in commercial pesticide formulations by Fourier transform infrared spectrometry. Journal of AOAC INTERNATIONAL, 2005, 88, 399-405.	1.5	1
118	Combining Pharmacokinetics and Vibrational Spectroscopy: MCR-ALS Hard-and-Soft Modelling of Drug Uptake In Vitro Using Tailored Kinetic Constraints. Cells, 2022, 11, 1555.	4.1	1
119	Metabolic characterization of PB60 and PB65, two peptidomimetics which notably facilitate the transport of heparin across the intestinal barrier. An activity of the Melius project. Toxicology Letters, 2010, 196, S269.	0.8	0
120	Advanced Spectroscopic Detectors for Identification and Quantification. , 2013, , 333-347.		0
121	PO-0414â€¦Plasma Metabolome In A Newborn Piglet Model For Asphyxia And Resuscitation. Archives of Disease in Childhood, 2014, 99, A381.1-A381.	1.9	0
122	Multiplexed Fourier Transform Infrared and Raman Imaging. Methods in Molecular Biology, 2021, 2350, 299-312.	0.9	0
123	Abstract 4369: Plasma metabolomic biomarkers for an early detection of colorectal cancer. , 2019, , .		0
124	ATR-Spin: an open-source 3D printed device for direct cytocentrifugation onto attenuated total reflectance crystals. Lab on A Chip, 2021, 21, 4743-4748.	6.0	0