

# Guillermo Quintãs

## List of Publications by Year in descending order

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124  
papers

2,973  
citations

196777

29  
h-index

274796

44  
g-index

128  
all docs

128  
docs citations

128  
times ranked

4619  
citing authors

#	ARTICLE	IF	CITATIONS
1	Noninvasive monitoring of evolving urinary metabolic patterns in neonatal encephalopathy. <i>Pediatric Research</i> , 2022, 91, 598-605.	1.1	9
2	A Novel UPLC-MS Metabolomic Analysis-Based Strategy to Monitor the Course and Extent of iPSC Differentiation to Hepatocytes. <i>Journal of Proteome Research</i> , 2022, , .	1.8	3
3	The effect of Holder pasteurization on the lipid and metabolite composition of human milk. <i>Food Chemistry</i> , 2022, 384, 132581.	4.2	8
4	Combining Pharmacokinetics and Vibrational Spectroscopy: MCR-ALS Hard-and-Soft Modelling of Drug Uptake In Vitro Using Tailored Kinetic Constraints. <i>Cells</i> , 2022, 11, 1555.	1.8	1
5	The Potential Role of Metabolomics in Drug-Induced Liver Injury (DILI) Assessment. <i>Metabolites</i> , 2022, 12, 564.	1.3	16
6	Direct Derivatization in Dried Blood Spots for Oxidized and Reduced Glutathione Quantification in Newborns. <i>Antioxidants</i> , 2022, 11, 1165.	2.2	4
7	Analysis of the Association between Fatigue and the Plasma Lipidomic Profile of Inflammatory Bowel Disease Patients. <i>Journal of Proteome Research</i> , 2021, 20, 381-392.	1.8	13
8	Effect of donor human milk on host-gut microbiota and metabolic interactions in preterm infants. <i>Clinical Nutrition</i> , 2021, 40, 1296-1309.	2.3	23
9	Metabolomic analysis to discriminate drug-induced liver injury (DILI) phenotypes. <i>Archives of Toxicology</i> , 2021, 95, 3049-3062.	1.9	24
10	A Reductive Metabolic Switch Protects Infants with Transposition of Great Arteries Undergoing Atrial Septostomy against Oxidative Stress. <i>Antioxidants</i> , 2021, 10, 1502.	2.2	2
11	ATR-FTIR spectroscopy for the routine quality control of exosome isolations. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2021, 217, 104401.	1.8	11
12	Multiplexed Fourier Transform Infrared and Raman Imaging. <i>Methods in Molecular Biology</i> , 2021, 2350, 299-312.	0.4	0
13	Extracting consistent biological information from functional results of metabolomic pathway analysis using the Mantel's test. <i>Analytica Chimica Acta</i> , 2021, 1187, 339173.	2.6	6
14	Factors that influence the quality of metabolomics data in in vitro cell toxicity studies: a systematic survey. <i>Scientific Reports</i> , 2021, 11, 22119.	1.6	9
15	ATR-Spin: an open-source 3D printed device for direct cytocentrifugation onto attenuated total reflectance crystals. <i>Lab on A Chip</i> , 2021, 21, 4743-4748.	3.1	0
16	Data mining Raman microspectroscopic responses of cells to drugs in vitro using multivariate curve resolution-alternating least squares. <i>Talanta</i> , 2020, 208, 120386.	2.9	10
17	Discriminant analysis and feature selection in mass spectrometry imaging using constrained repeated random sampling - Cross validation (CORRS-CV). <i>Analytica Chimica Acta</i> , 2020, 1097, 30-36.	2.6	13
18	Metabolomic profiling in neuroblastoma. <i>Pediatric Blood and Cancer</i> , 2020, 67, e28113.	0.8	5

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19	Immunosuppressive profiles in liquid biopsy at diagnosis predict response to neoadjuvant chemotherapy in triple-negative breast cancer. <i>European Journal of Cancer</i> , 2020, 139, 119-134.	1.3	26
20	Toward Rapid Screening of Liver Grafts at the Operating Room Using Mid-infrared Spectroscopy. <i>Analytical Chemistry</i> , 2020, 92, 14542-14549.	3.2	8
21	Metabolic Phenotypes of Hypoxic-Ischemic Encephalopathy with Normal vs. Pathologic Magnetic Resonance Imaging Outcomes. <i>Metabolites</i> , 2020, 10, 109.	1.3	14
22	Urine metabolomic analysis for monitoring internal load in professional football players. <i>Metabolomics</i> , 2020, 16, 45.	1.4	19
23	Comparing Targeted vs. Untargeted MS2 Data-Dependent Acquisition for Peak Annotation in LC-MS Metabolomics. <i>Metabolites</i> , 2020, 10, 126.	1.3	29
24	Current Practice in Untargeted Human Milk Metabolomics. <i>Metabolites</i> , 2020, 10, 43.	1.3	21
25	Monitoring of system conditioning after blank injections in untargeted UPLC-MS metabolomic analysis. <i>Scientific Reports</i> , 2019, 9, 9822.	1.6	26
26	Urinary Metabolic Signatures Detect Recurrences in Non-Muscle Invasive Bladder Cancer. <i>Cancers</i> , 2019, 11, 914.	1.7	19
27	Troubleshooting in Large-Scale LC-ToF-MS Metabolomics Analysis: Solving Complex Issues in Big Cohorts. <i>Metabolites</i> , 2019, 9, 247.	1.3	13
28	Integrative Metabolomic and Transcriptomic Analysis for the Study of Bladder Cancer. <i>Cancers</i> , 2019, 11, 686.	1.7	31
29	Adrenic acid non-enzymatic peroxidation products in biofluids of moderate preterm infants. <i>Free Radical Biology and Medicine</i> , 2019, 142, 107-112.	1.3	10
30	High and ultra-high definition of infrared spectral histopathology gives an insight into chemical environment of lung metastases in breast cancer. <i>Journal of Biophotonics</i> , 2019, 12, e201800345.	1.1	18
31	Abstract 4369: Plasma metabolomic biomarkers for an early detection of colorectal cancer. , 2019, , .		0
32	Model selection for within-batch effect correction in UPLC-MS metabolomics using quality control - Support vector regression. <i>Analytica Chimica Acta</i> , 2018, 1026, 62-68.	2.6	32
33	Fast quantification of bovine milk proteins employing external cavity-quantum cascade laser spectroscopy. <i>Food Chemistry</i> , 2018, 252, 22-27.	4.2	19
34	Evaluation of batch effect elimination using quality control replicates in LC-MS metabolite profiling. <i>Analytica Chimica Acta</i> , 2018, 1019, 38-48.	2.6	42
35	Liquid Chromatography-FTIR. <i>Liquid Chromatography-Fourier Transform Infrared</i> . , 2018, , 75-75.		2
36	On-Capillary Surface-Enhanced Raman Spectroscopy: Determination of Glutathione in Whole Blood Microsamples. <i>Analytical Chemistry</i> , 2018, 90, 9093-9100.	3.2	40

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37	Non-invasive prediction of NAFLD severity: a comprehensive, independent validation of previously postulated serum microRNA biomarkers. <i>Scientific Reports</i> , 2018, 8, 10606.	1.6	52
38	Assessment of discriminant models in infrared imaging using constrained repeated random sampling â€“ Cross validation. <i>Analytica Chimica Acta</i> , 2018, 1033, 156-164.	2.6	17
39	Data Quality Assessment in Untargeted LC-MS Metabolomics. <i>Comprehensive Analytical Chemistry</i> , 2018, 82, 137-164.	0.7	6
40	Bladder cancer recurrence surveillance by urine metabolomics analysis. <i>Scientific Reports</i> , 2018, 8, 9172.	1.6	54
41	Assessment of phospholipid synthesis related biomarkers for perinatal asphyxia: a piglet study. <i>Scientific Reports</i> , 2017, 7, 40315.	1.6	16
42	External cavity-quantum cascade laser (EC-QCL) spectroscopy for protein analysis in bovine milk. <i>Analytica Chimica Acta</i> , 2017, 963, 99-105.	2.6	22
43	Plasma metabolite score correlates with Hypoxia time in a newly born piglet model for asphyxia. <i>Redox Biology</i> , 2017, 12, 1-7.	3.9	25
44	Novel free-radical mediated lipid peroxidation biomarkers in newborn plasma. <i>Analytica Chimica Acta</i> , 2017, 996, 88-97.	2.6	30
45	Advanced IR and Raman detectors for identification and quantification. , 2017, , 463-477.		3
46	Plasma sample based analysis of gastric cancer progression using targeted metabolomics. <i>Scientific Reports</i> , 2017, 7, 17774.	1.6	56
47	Metabolomic Analysis of Gastric Cancer Progression within the Correaâ€™s Cascade Using Ultraperformance Liquid Chromatographyâ€™Mass Spectrometry. <i>Journal of Proteome Research</i> , 2016, 15, 2729-2738.	1.8	32
48	Changes of the plasma metabolome of newly born piglets subjected to postnatal hypoxia and resuscitation with air. <i>Pediatric Research</i> , 2016, 80, 284-292.	1.1	24
49	Detection of prostate cancer using a voltammetric electronic tongue. <i>Analyst, The</i> , 2016, 141, 4562-4567.	1.7	18
50	Surface enhanced Raman spectroscopic direct determination of low molecular weight biothiols in umbilical cord whole blood. <i>Analyst, The</i> , 2016, 141, 2165-2174.	1.7	24
51	Application of Discriminant Analysis and Cross-Validation on Proteomics Data. <i>Methods in Molecular Biology</i> , 2016, 1362, 175-184.	0.4	14
52	Urinary Lipid Peroxidation Byproducts: Are They Relevant for Predicting Neonatal Morbidity in Preterm Infants?. <i>Antioxidants and Redox Signaling</i> , 2015, 23, 178-184.	2.5	53
53	Analysis of multi-source metabolomic data using joint and individual variation explained (JIVE). <i>Analyst, The</i> , 2015, 140, 4521-4529.	1.7	21
54	Intra-batch effect correction in liquid chromatography-mass spectrometry using quality control samples and support vector regression (QC-SVRC). <i>Analyst, The</i> , 2015, 140, 7810-7817.	1.7	96

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55	Assessment of the statistical significance of classifications in infrared spectroscopy based diagnostic models. <i>Analyst, The</i> , 2015, 140, 2422-2427.	1.7	19
56	Assessment of Oxidative Damage to Proteins and DNA in Urine of Newborn Infants by a Validated UPLC-MS/MS Approach. <i>PLoS ONE</i> , 2014, 9, e93703.	1.1	28
57	Metabolic adaptation and neuroprotection differ in the retina and choroid in a piglet model of acute postnatal hypoxia. <i>Pediatric Research</i> , 2014, 76, 127-134.	1.1	12
58	PO-0414â€¦Plasma Metabolome In A Newborn Piglet Model For Asphyxia And Resuscitation. <i>Archives of Disease in Childhood</i> , 2014, 99, A381.1-A381.	1.0	0
59	Analysis of lipid peroxidation biomarkers in extremely low gestational age neonate urines by UPLC-MS/MS. <i>Analytical and Bioanalytical Chemistry</i> , 2014, 406, 4345-4356.	1.9	40
60	High performance liquid chromatography with mid-infrared detection based on a broadly tunable quantum cascade laser. <i>Analyst, The</i> , 2014, 139, 2057.	1.7	24
61	Towards the potential use of <sup>1</sup> H NMR spectroscopy in urine samples for prostate cancer detection. <i>Analyst, The</i> , 2014, 139, 3875-3878.	1.7	15
62	Detection of batch effects in liquid chromatography-mass spectrometry metabolomic data using guided principal component analysis. <i>Talanta</i> , 2014, 130, 442-448.	2.9	27
63	Infrared biospectroscopy for a fast qualitative evaluation of sample preparation in metabolomics. <i>Talanta</i> , 2014, 127, 181-190.	2.9	9
64	Prolonging in utero-like oxygenation after birth diminishes oxidative stress in the lung and brain of mice pups. <i>Redox Biology</i> , 2013, 1, 297-303.	3.9	10
65	Advanced Spectroscopic Detectors for Identification and Quantification. , 2013, , 333-347.		0
66	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. <i>Toxicology in Vitro</i> , 2013, 27, 1357-1376.	1.1	31
67	Evaluation of the effect of chance correlations on variable selection using Partial Least Squares-Discriminant Analysis. <i>Talanta</i> , 2013, 116, 835-840.	2.9	21
68	Modified locally weightedâ€”Partial least squares regression improving clinical predictions from infrared spectra of human serum samples. <i>Talanta</i> , 2013, 107, 368-375.	2.9	30
69	Dichloro-dihydro-fluorescein diacetate (DCFH-DA) assay: A quantitative method for oxidative stress assessment of nanoparticle-treated cells. <i>Toxicology in Vitro</i> , 2013, 27, 954-963.	1.1	349
70	Improving the performance of hollow waveguide-based infrared gas sensors via tailored chemometrics. <i>Analytical and Bioanalytical Chemistry</i> , 2013, 405, 8223-8232.	1.9	10
71	Atmospheric Compensation in Fourier Transform Infrared (FT-IR) Spectra of Clinical Samples. <i>Applied Spectroscopy</i> , 2013, 67, 1339-1342.	1.2	11
72	Metabolomic Analysis of the Effect of Postnatal Hypoxia on the Retina in a Newly Born Piglet Model. <i>PLoS ONE</i> , 2013, 8, e66540.	1.1	19

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73	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. <i>Talanta</i> , 2012, 99, 566-573.	2.9	35
74	Predicting survival of patients with hypocellular myelodysplastic syndrome. <i>Cancer</i> , 2012, 118, 4462-4470.	2.0	38
75	Direct determination of polymerised triacylglycerides in deep-frying vegetable oil by near infrared spectroscopy using Partial Least Squares regression. <i>Food Chemistry</i> , 2012, 131, 353-359.	4.2	33
76	Chemometric approaches to improve PLS-DA model outcome for predicting human non-alcoholic fatty liver disease using UPLC-MS as a metabolic profiling tool. <i>Metabolomics</i> , 2012, 8, 86-98.	1.4	54
77	Background Correction and Multivariate Curve Resolution of Online Liquid Chromatography with Infrared Spectrometric Detection. <i>Analytical Chemistry</i> , 2011, 83, 4855-4862.	3.2	39
78	Science based calibration for the extraction of analyte-specific HPLC-DAD chromatograms in environmental analysis. <i>Talanta</i> , 2011, 83, 1158-1165.	2.9	5
79	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. <i>Analytical and Bioanalytical Chemistry</i> , 2011, 399, 1305-1314.	1.9	19
80	Monitoring of Polymerized Triglycerides in Deep-Frying Oil by On-Line GPC-FTIR Spectrometry Using the Science Based Calibration Multivariate Approach. <i>Chromatographia</i> , 2010, 71, 201-209.	0.7	14
81	Direct determination of polymerized triglycerides in deep-frying olive oil by attenuated total reflectance Fourier transform infrared spectroscopy using partial least squares regression. <i>Analytical and Bioanalytical Chemistry</i> , 2010, 397, 861-869.	1.9	16
82	High performance liquid chromatography with on-line dual quantum cascade laser detection for the determination of carbohydrates, alcohols and organic acids in wine and grape juice. <i>Applied Physics B: Lasers and Optics</i> , 2010, 99, 833-840.	1.1	23
83	Recent advances in on-line liquid chromatography - infrared spectrometry (LC-IR). <i>TrAC - Trends in Analytical Chemistry</i> , 2010, 29, 544-552.	5.8	27
84	Analytical potential of mid-infrared detection in capillary electrophoresis and liquid chromatography: A review. <i>Analytica Chimica Acta</i> , 2010, 679, 31-42.	2.6	39
85	Cubic smoothing splines background correction in on-line liquid chromatography Fourier transform infrared spectrometry. <i>Journal of Chromatography A</i> , 2010, 1217, 6733-6741.	1.8	12
86	Application of point-to-point matching algorithms for background correction in on-line liquid chromatography Fourier transform infrared spectrometry (LC-FTIR). <i>Talanta</i> , 2010, 80, 1771-1776.	2.9	15
87	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. <i>Toxicology Letters</i> , 2010, 196, S269.	0.4	0
88	Chemometric extraction of analyte-specific chromatograms in on-line gradient LC-infrared spectrometry. <i>Journal of Separation Science</i> , 2009, 32, 4089-4095.	1.3	13
89	Determination of enzyme activity inhibition by FTIR spectroscopy on the example of fructose biphosphatase. <i>Analytical and Bioanalytical Chemistry</i> , 2009, 394, 2137-2144.	1.9	10
90	New background correction approach based on polynomial regressions for on-line liquid chromatography Fourier transform infrared spectrometry. <i>Journal of Chromatography A</i> , 2009, 1216, 3122-3130.	1.8	26

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91	On-Line Fourier Transform Infrared Spectrometric Detection in Gradient Capillary Liquid Chromatography Using Nanoliter-Flow Cells. <i>Analytical Chemistry</i> , 2009, 81, 3746-3753.	3.2	24
92	Procedure for Automated Background Correction in Flow Systems with Infrared Spectroscopic Detection and Changing Liquid-Phase Composition. <i>Applied Spectroscopy</i> , 2009, 63, 1363-1369.	1.2	7
93	New cut-off criterion for uninformative variable elimination in multivariate calibration of near-infrared spectra for the determination of heroin in illicit street drugs. <i>Analytica Chimica Acta</i> , 2008, 630, 150-160.	2.6	31
94	Determination of glycolic acid in cosmetics by online liquid chromatographyâ€“Fourier transform infrared spectrometry. <i>Analytical and Bioanalytical Chemistry</i> , 2008, 392, 1383-1389.	1.9	12
95	Determination of critical eluent composition for polyethyleneglycols using on-line liquid chromatographyâ€“Fourier transform infrared spectrometry. <i>Analytica Chimica Acta</i> , 2008, 624, 278-285.	2.6	17
96	Univariate method for background correction in liquid chromatographyâ€“Fourier transform infrared spectrometry. <i>Journal of Chromatography A</i> , 2008, 1190, 102-109.	1.8	25
97	On-line gel permeation chromatographyâ€“attenuated total reflectanceâ€“Fourier transform infrared determination of lecithin and soybean oil in dietary supplements. <i>Journal of Chromatography A</i> , 2008, 1185, 71-77.	1.8	35
98	First-order derivative resolution of overlapped PAH peaks with common mass spectra in gas chromatographyâ€“mass spectrometry. <i>Talanta</i> , 2008, 74, 747-752.	2.9	6
99	Towards minimization of chlorinated solvents consume in Fourier transform infrared spectroscopy determination of Propamocarb in pesticide formulations. <i>Talanta</i> , 2008, 75, 339-343.	2.9	2
100	Determination of lecithin and soybean oil in dietary supplements using partial least squaresâ€“Fourier transform infrared spectroscopy. <i>Talanta</i> , 2008, 77, 229-234.	2.9	31
101	On-line gradient liquid chromatographyâ€“Fourier transform infrared spectrometry determination of sugars in beverages using chemometric background correction. <i>Talanta</i> , 2008, 77, 779-785.	2.9	20
102	Firstâ€“Derivative Fourierâ€“Transform Infrared Determination of Oxadiazon in Commercial Herbicide Formulations. <i>Spectroscopy Letters</i> , 2008, 41, 1-8.	0.5	8
103	HPLC determination of oxadiazon in commercial pesticide formulations. <i>Journal of the Brazilian Chemical Society</i> , 2008, 19, 1394-1398.	0.6	6
104	Automated sample preparation and analysis using a sequential-injectionâ€“capillary electrophoresis (SIâ€“CE) interface. <i>Analyst</i> , The, 2006, 131, 739-744.	1.7	40
105	Determination of PAHs in airborne particles by accelerated solvent extraction and large-volume injectionâ€“gas chromatographyâ€“mass spectrometry. <i>Talanta</i> , 2006, 69, 807-815.	2.9	63
106	Development of a simple and low cost device for vapour phase Fourier Transform Infrared spectrometry determination of ethanol in mouthwashes. <i>Analytica Chimica Acta</i> , 2006, 569, 238-243.	2.6	10
107	On-line capillary electrophoresis FTIR detection for the separation and characterization of proteins. <i>Vibrational Spectroscopy</i> , 2006, 42, 392-396.	1.2	6
108	Determination of Peroxide-Based Explosives Using Liquid Chromatography with On-Line Infrared Detection. <i>Analytical Chemistry</i> , 2006, 78, 8150-8155.	3.2	82

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109	On-line monitoring of pH junctions in capillary electrophoresis using Fourier transform infrared spectrometry. <i>Analytical and Bioanalytical Chemistry</i> , 2006, 387, 287-292.	1.9	6
110	Determination of acrylamide in foods by pressurized fluid extraction and liquid chromatography-tandem mass spectrometry used for a survey of Spanish cereal-based foods. <i>Food Additives and Contaminants</i> , 2006, 23, 237-244.	2.0	44
111	Mid-infrared and Raman spectrometry for quality control of pesticide formulations. <i>TrAC - Trends in Analytical Chemistry</i> , 2005, 24, 772-781.	5.8	51
112	A validated and fast procedure for FTIR determination of Cypermethrin and Chlorpyrifos. <i>Talanta</i> , 2005, 67, 634-639.	2.9	39
113	FTIR Approaches for Diuron Determination in Commercial Pesticide Formulations. <i>Journal of Agricultural and Food Chemistry</i> , 2005, 53, 5842-5847.	2.4	17
114	Determination of pirimicarb and endosulfan in commercial pesticide formulations by Fourier transform infrared spectrometry. <i>Journal of AOAC INTERNATIONAL</i> , 2005, 88, 399-405.	0.7	1
115	Fourier transform infrared determination of imidacloprid in pesticide formulations. <i>Journal of the Brazilian Chemical Society</i> , 2004, 15, 307-312.	0.6	26
116	FT-Raman determination of Mepiquat chloride in agrochemical products. <i>Vibrational Spectroscopy</i> , 2004, 36, 41-46.	1.2	12
117	Fourier transform infrared spectrometric determination of Malathion in pesticide formulations. <i>Analytica Chimica Acta</i> , 2004, 502, 213-220.	2.6	25
118	Determination of cyromazine in pesticide commercial formulations by vibrational spectrometric procedures. <i>Analytica Chimica Acta</i> , 2004, 524, 257-264.	2.6	25
119	FT-Raman spectrometry determination of Malathion in pesticide formulations. <i>Talanta</i> , 2004, 63, 345-350.	2.9	30
120	Simultaneous determination of Folpet and Metalaxyl in pesticide formulations by flow injection Fourier transform infrared spectrometry. <i>Analytica Chimica Acta</i> , 2003, 480, 11-21.	2.6	34
121	Fourier transform infrared determination of Fluometuron in pesticide formulations. <i>Vibrational Spectroscopy</i> , 2003, 31, 63-69.	1.2	15
122	An Infrared Method, with Reduced Solvent Consumption, for the Determination of Chlorsulfuron in Pesticide Formulations. <i>Spectroscopy Letters</i> , 2003, 36, 515-529.	0.5	2
123	Determination of caffeine in tea samples by Fourier transform infrared spectrometry. <i>Analytical and Bioanalytical Chemistry</i> , 2002, 374, 561-565.	1.9	28
124	Fourier transform infrared spectrometric strategies for the determination of Buprofezin in pesticide formulations. <i>Analytica Chimica Acta</i> , 2002, 468, 81-90.	2.6	29