## Julien Boccard

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	A consensus orthogonal partial least squares discriminant analysis (OPLS-DA) strategy for multiblock Omics data fusion. Analytica Chimica Acta, 2013, 769, 30-39.	5.4	246
2	Antimitotic and Antiproliferative Activities of Chalcones: Forward Structure–Activity Relationship. Journal of Medicinal Chemistry, 2008, 51, 2307-2310.	6.4	166
3	Knowledge discovery in metabolomics: An overview of MS data handling. Journal of Separation Science, 2010, 33, 290-304.	2.5	158
4	Metabolomics reveals herbivoreâ€induced metabolites of resistance and susceptibility in maize leaves and roots. Plant, Cell and Environment, 2013, 36, 621-639.	5.7	149
5	Metabolomic analysis of urine samples by UHPLC-QTOF-MS: Impact of normalization strategies. Analytica Chimica Acta, 2017, 955, 27-35.	5.4	129
6	Analysis of basic compounds by supercritical fluid chromatography: Attempts to improve peak shape and maintain mass spectrometry compatibility. Journal of Chromatography A, 2012, 1262, 205-213.	3.7	101
7	Rumen microbial communities influence metabolic phenotypes in lambs. Frontiers in Microbiology, 2015, 6, 1060.	3.5	98
8	Optimized liquid chromatography–mass spectrometry approach for the isolation of minor stress biomarkers in plant extracts and their identification by capillary nuclear magnetic resonance. Journal of Chromatography A, 2008, 1180, 90-98.	3.7	97
9	UPLC–TOF-MS for plant metabolomics: A sequential approach for wound marker analysis in Arabidopsis thaliana. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2008, 871, 261-270.	2.3	96
10	Differentiation of lemon essential oil based on volatile and non-volatile fractions with various analytical techniques: a metabolomic approach. Food Chemistry, 2014, 143, 325-335.	8.2	92
11	Harnessing the complexity of metabolomic data with chemometrics. Journal of Chemometrics, 2014, 28, 1-9.	1.3	90
12	Implementation of liquid chromatography–high resolution mass spectrometry methods for untargeted metabolomic analyses of biological samples: A tutorial. Analytica Chimica Acta, 2020, 1105, 28-44.	5.4	83
13	Quantification of glucuronidated and sulfated steroids in human urine by ultra-high pressure liquid chromatography quadrupole time-of-flight mass spectrometry. Analytical and Bioanalytical Chemistry, 2011, 400, 503-516.	3.7	82
14	Evaluation of steroidomics by liquid chromatography hyphenated to mass spectrometry as a powerful analytical strategy for measuring human steroid perturbations. Journal of Chromatography A, 2016, 1430, 97-112.	3.7	80
15	Systematic comparison of sensitivity between hydrophilic interaction liquid chromatography and reversed phase liquid chromatography coupled with mass spectrometry. Journal of Chromatography A, 2013, 1312, 49-57.	3.7	73
16	Profiling of steroid metabolites after transdermal and oral administration of testosterone by ultra-high pressure liquid chromatography coupled to quadrupole time-of-flight mass spectrometry. Journal of Steroid Biochemistry and Molecular Biology, 2013, 138, 222-235.	2.5	67
17	A steroidomic approach for biomarkers discovery in doping control. Forensic Science International, 2011, 213, 85-94.	2.2	66
18	Exploring Omics data from designed experiments using analysis of variance multiblock Orthogonal Partial Least Squares. Analytica Chimica Acta, 2016, 920, 18-28.	5.4	63

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19	Metabolite profiling of plant extracts by ultra-high-pressure liquid chromatography at elevated temperature coupled to time-of-flight mass spectrometry. Journal of Chromatography A, 2009, 1216, 5660-5668.	3.7	61
20	Prediction of retention time in reversed-phase liquid chromatography as a tool for steroid identification. Analytica Chimica Acta, 2016, 916, 8-16.	5.4	58
21	Longitudinal monitoring of endogenous steroids in human serum by UHPLC-MS/MS as a tool to detect testosterone abuse in sports. Analytical and Bioanalytical Chemistry, 2016, 408, 705-719.	3.7	57
22	Ultra-high performance supercritical fluid chromatography coupled with quadrupole-time-of-flight mass spectrometry as a performing tool for bioactive analysis. Journal of Chromatography A, 2016, 1450, 101-111.	3.7	56
23	Targeted metabolomics shows plasticity in the evolution of signaling lipids and uncovers old and new endocannabinoids in the plant kingdom. Scientific Reports, 2017, 7, 41177.	3.3	52
24	Human urinary biomarkers of dioxin exposure: Analysis by metabolomics and biologically driven data dimensionality reduction. Toxicology Letters, 2014, 230, 234-243.	0.8	51
25	Development of a twoâ€step screening ESIâ€TOFâ€MS method for rapid determination of significant stressâ€induced metabolome modifications in plant leaf extracts: The wound response in <i>Arabidopsis thaliana</i> as a case study. Journal of Separation Science, 2007, 30, 2268-2278.	2.5	46
26	Analytical aspects in doping control: Challenges and perspectives. Forensic Science International, 2011, 213, 49-61.	2.2	46
27	Metabolomics approach reveals disruption of metabolic pathways in the marine bivalve Mytilus galloprovincialis exposed to a WWTP effluent extract. Science of the Total Environment, 2020, 712, 136551.	8.0	45
28	Retention time prediction for dereplication of natural products (CxHyOz) in LC–MS metabolite profiling. Phytochemistry, 2014, 108, 196-207.	2.9	44
29	Steroid profiling in H295R cells to identify chemicals potentially disrupting the production of adrenal steroids. Toxicology, 2017, 381, 51-63.	4.2	42
30	Breast cancer resistance protein (BCRP/ABCG2): New inhibitors and QSAR studies by a 3D linear solvation energy approach. European Journal of Pharmaceutical Sciences, 2009, 38, 39-46.	4.0	41
31	From a single steroid to the steroidome: Trends and analytical challenges. Journal of Steroid Biochemistry and Molecular Biology, 2021, 206, 105797.	2.5	41
32	Dynamics of Metabolite Induction in Fungal Co-cultures by Metabolomics at Both Volatile and Non-volatile Levels. Frontiers in Microbiology, 2018, 9, 72.	3.5	40
33	A scoring approach for multi-platform acquisition in metabolomics. Journal of Chromatography A, 2019, 1592, 47-54.	3.7	40
34	Structured plant metabolomics for the simultaneous exploration of multiple factors. Scientific Reports, 2016, 6, 37390.	3.3	39
35	Multivariate data analysis of rapid LC-TOF/MS experiments from Arabidopsis thaliana stressed by wounding. Chemometrics and Intelligent Laboratory Systems, 2007, 86, 189-197.	3.5	35
36	Mass spectrometryâ€based metabolomics oriented by correlation analysis for woundâ€induced molecule discovery: identification of a novel jasmonate glucoside. Phytochemical Analysis, 2010, 21, 95-101.	2.4	35

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37	Comprehensive Examination of the Mouse Lung Metabolome Following <i>Mycobacterium tuberculosis</i> Infection Using a Multiplatform Mass Spectrometry Approach. Journal of Proteome Research, 2020, 19, 2053-2070.	3.7	35
38	Quantitative monitoring of tamoxifen in human plasma extended to 40 metabolites using liquid-chromatography high-resolution mass spectrometry: new investigation capabilities for clinical pharmacology. Analytical and Bioanalytical Chemistry, 2014, 406, 2627-2640.	3.7	34
39	High-resolution mass spectrometry as an alternative detection method to tandem mass spectrometry for the analysis of endogenous steroids in serum. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2017, 1052, 34-42.	2.3	34
40	Applicability of Supercritical fluid chromatography–Mass spectrometry to metabolomics. Il–Assessment of a comprehensive library of metabolites and evaluation of biological matrices. Journal of Chromatography A, 2020, 1620, 461021.	3.7	34
41	A 3D linear solvation energy model to quantify the affinity of flavonoid derivatives toward P-glycoprotein. European Journal of Pharmaceutical Sciences, 2009, 36, 254-264.	4.0	33
42	Method development for pharmaceutics: Some solutions for tuning selectivity in reversed phase and hydrophilic interaction liquid chromatography. Journal of Pharmaceutical and Biomedical Analysis, 2012, 63, 95-105.	2.8	33
43	MS-based plant metabolomic approaches for biomarker discovery. Natural Product Communications, 2009, 4, 1417-30.	0.5	31
44	Approaches in metabolomics for regulatory toxicology applications. Analyst, The, 2021, 146, 1820-1834.	3.5	30
45	Longitudinal evaluation of multiple biomarkers for the detection of testosterone gel administration in women with normal menstrual cycle. Drug Testing and Analysis, 2022, 14, 833-850.	2.6	29
46	Systematic evaluation of matrix effects in hydrophilic interaction chromatography versus reversed phase liquid chromatography coupled to mass spectrometry. Journal of Chromatography A, 2016, 1439, 42-53.	3.7	28
47	Optimized selection of liquid chromatography conditions for wide range analysis of natural compounds. Journal of Chromatography A, 2017, 1504, 91-104.	3.7	28
48	Evaluation and identification of dioxin exposure biomarkers in human urine by high-resolution metabolomics, multivariate analysis and in vitro synthesis. Toxicology Letters, 2016, 240, 22-31.	0.8	27
49	Unravelling the effects of multiple experimental factors in metabolomics, analysis of human neural cells with hydrophilic interaction liquid chromatography hyphenated to high resolution mass spectrometry. Journal of Chromatography A, 2017, 1527, 53-60.	3.7	27
50	Comprehensive profiling and marker identification in non-volatile citrus oil residues by mass spectrometry and nuclear magnetic resonance. Food Chemistry, 2014, 150, 235-245.	8.2	26
51	MS-based Plant Metabolomic Approaches for Biomarker Discovery. Natural Product Communications, 2009, 4, 1934578X0900401.	0.5	25
52	Untargeted profiling of urinary steroid metabolites after testosterone ingestion: opening new perspectives for antidoping testing. Bioanalysis, 2014, 6, 2523-2536.	1.5	25
53	Enhanced metabolite annotation via dynamic retention time prediction: Steroidogenesis alterations as a case study. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2017, 1071, 11-18.	2.3	25
54	Steroidomic Footprinting Based on Ultra-High Performance Liquid Chromatography Coupled with Qualitative and Quantitative High-Resolution Mass Spectrometry for the Evaluation of Endocrine Disrupting Chemicals in H295R Cells. Chemical Research in Toxicology, 2015, 28, 955-966.	3.3	24

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55	An Integrative Multi-Omics Workflow to Address Multifactorial Toxicology Experiments. Metabolites, 2019, 9, 79.	2.9	24
56	Steroid profiling by UHPLC-MS/MS in dried blood spots collected from healthy women with and without testosterone gel administration. Journal of Pharmaceutical and Biomedical Analysis, 2021, 204, 114280.	2.8	24
57	Standard machine learning algorithms applied to UPLC-TOF/MS metabolic fingerprinting for the discovery of wound biomarkers in Arabidopsis thaliana. Chemometrics and Intelligent Laboratory Systems, 2010, 104, 20-27.	3.5	23
58	Metabolomics in chronic kidney disease: Strategies for extended metabolome coverage. Journal of Pharmaceutical and Biomedical Analysis, 2018, 161, 313-325.	2.8	23
59	Steroidomics for highlighting novel serum biomarkers of testosterone doping. Bioanalysis, 2019, 11, 1169-1185.	1.5	23
60	Assessing Susceptibility to Epilepsy in Three Rat Strains Using Brain Metabolic Profiling Based on HRMAS NMR Spectroscopy and Chemometrics. Journal of Proteome Research, 2015, 14, 2177-2189.	3.7	21
61	Metabotypes of Pseudomonas aeruginosa Correlate with Antibiotic Resistance, Virulence and Clinical Outcome in Cystic Fibrosis Chronic Infections. Metabolites, 2021, 11, 63.	2.9	20
62	Multifactorial Analysis of Environmental Metabolomic Data in Ecotoxicology: Wild Marine Mussel Exposed to WWTP Effluent as a Case Study. Metabolites, 2020, 10, 269.	2.9	19
63	Multi-way PLS for discrimination: Compact form equivalent to the tri-linear PLS2 procedure and its monotony convergence. Chemometrics and Intelligent Laboratory Systems, 2014, 133, 25-32.	3.5	18
64	DynaStl: A Dynamic Retention Time Database for Steroidomics. Metabolites, 2019, 9, 85.	2.9	18
65	Steroid profiles in both blood serum and seminal plasma are not correlated and do not reflect sperm quality: Study on the male reproductive health of fifty young Swiss men. Clinical Biochemistry, 2018, 62, 39-46.	1.9	16
66	Development and validation of an UHPLC–MS/MS method for extended serum steroid profiling in female populations. Bioanalysis, 2020, 12, 753-768.	1.5	16
67	Statistical Correlations between HPLC Activity-Based Profiling Results and NMR/MS Microfraction Data to Deconvolute Bioactive Compounds in Mixtures. Molecules, 2016, 21, 259.	3.8	15
68	Toward a better understanding of chronic kidney disease with complementary chromatographic methods hyphenated with mass spectrometry for improved polar metabolome coverage. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2019, 1116, 9-18.	2.3	15
69	An integrated metabolomics and proteogenomics approach reveals molecular alterations following carbamazepine exposure in the male mussel Mytilus galloprovincialis. Chemosphere, 2022, 286, 131793.	8.2	15
70	Integrating metabolomic data from multiple analytical platforms for a comprehensive characterisation of lemon essential oils. Flavour and Fragrance Journal, 2015, 30, 131-138.	2.6	14
71	Exploring blood alterations in chronic kidney disease and haemodialysis using metabolomics. Scientific Reports, 2020, 10, 19502.	3.3	14
72	Steroid profile analysis by LC-HRMS in human seminal fluid. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2020, 1136, 121929.	2.3	13

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73	Neuroinflammatory Response to TNFα and IL1β Cytokines Is Accompanied by an Increase in Glycolysis in Human Astrocytes In Vitro. International Journal of Molecular Sciences, 2021, 22, 4065.	4.1	13
74	Phenotypic and molecular characterization of proliferating and differentiated GnRH-expressing GnV-3 cells. Molecular and Cellular Endocrinology, 2011, 332, 97-105.	3.2	12
75	Methods for Doping Detection. Frontiers of Hormone Research, 2016, 47, 153-167.	1.0	12
76	Cultivar, site or harvest date: the gordian knot of wine terroir. Metabolomics, 2020, 16, 52.	3.0	12
77	CD40-CD40 Ligand Disruption Does Not Prevent Hyperoxia-Induced Injury. American Journal of Pathology, 2002, 160, 67-71.	3.8	11
78	IEF pattern classificationâ€derived criteria for the identification of epoetinâ€Î´ in urine. Electrophoresis, 2010, 31, 1918-1924.	2.4	11
79	Analysis of experimental design with multivariate response: A contribution using multiblock techniques. Chemometrics and Intelligent Laboratory Systems, 2011, 106, 65-72.	3.5	11
80	Mass Spectrometry Metabolomic Data Handling for Biomarker Discovery. , 2013, , 425-445.		11
81	High-throughput identification of monoclonal antibodies after compounding by UV spectroscopy coupled to chemometrics analysis. Analytical and Bioanalytical Chemistry, 2016, 408, 5915-5924.	3.7	11
82	UHPLC-HRMS Analysis for Steroid Profiling in Serum (Steroidomics). Methods in Molecular Biology, 2018, 1738, 261-278.	0.9	11
83	Choosing an Optimal Sample Preparation in Caulobacter crescentus for Untargeted Metabolomics Approaches. Metabolites, 2019, 9, 193.	2.9	11
84	In vitro models to study insulin and glucocorticoids modulation of trimethyltin (TMT)-induced neuroinflammation and neurodegeneration, and in vivo validation in db/db mice. Archives of Toxicology, 2019, 93, 1649-1664.	4.2	11
85	Supercritical fluid chromatography–mass spectrometry in routine anti-doping analyses: Estimation of retention time variability under reproducible conditions. Journal of Chromatography A, 2020, 1616, 460780.	3.7	11
86	Insights on the Structural and Metabolic Resistance of Potato (Solanum tuberosum) Cultivars to Tuber Black Dot (Colletotrichum coccodes). Frontiers in Plant Science, 2020, 11, 1287.	3.6	11
87	Multi-way PLS regression: Monotony convergence of tri-linear PLS2 and optimality of parameters. Computational Statistics and Data Analysis, 2015, 83, 129-139.	1.2	10
88	Removal of batch effects using stratified subsampling of metabolomic data for in vitro endocrine disruptors screening. Talanta, 2019, 195, 77-86.	5.5	10
89	Profiling of anabolic androgenic steroids and selective androgen receptor modulators for interference with adrenal steroidogenesis. Biochemical Pharmacology, 2020, 172, 113781.	4.4	10
90	Iterative weighting of multiblock data in the orthogonal partial least squares framework. Analytica Chimica Acta, 2014, 813, 25-34.	5.4	9

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91	Evaluation of Different Tandem MS Acquisition Modes to Support Metabolite Annotation in Human Plasma Using Ultra High-Performance Liquid Chromatography High-Resolution Mass Spectrometry for Untargeted Metabolomics. Metabolites, 2020, 10, 464.	2.9	9
92	Standardized LC×LC-ELSD Fractionation Procedure for the Identification of Minor Bioactives via the Enzymatic Screening of Natural Extracts. Journal of Natural Products, 2016, 79, 2856-2864.	3.0	7
93	Processing of NMR and MS metabolomics data using chemometrics methods: a global tool for fungi biotransformation reactions monitoring. Metabolomics, 2019, 15, 107.	3.0	7
94	Combining the advantages of multilevel and orthogonal partial least squares data analysis for longitudinal metabolomics: Application to kidney transplantation. Analytica Chimica Acta, 2020, 1099, 26-38.	5.4	7
95	Network principal component analysis: a versatile tool for the investigation of multigroup and multiblock datasets. Bioinformatics, 2021, 37, 1297-1303.	4.1	6
96	Protein pathway analysis to study development-dependent effects of acute and repeated trimethyltin (TMT) treatments in 3D rat brain cell cultures. Toxicology in Vitro, 2019, 60, 281-292.	2.4	5
97	Gaining Insights Into Metabolic Networks Using Chemometrics and Bioinformatics: Chronic Kidney Disease as a Clinical Model. Frontiers in Molecular Biosciences, 2021, 8, 682559.	3.5	5
98	Wipe-sampling procedure optimisation for the determination of 23 antineoplastic drugs used in the hospital pharmacy. European Journal of Hospital Pharmacy, 2021, 28, 94-99.	1.1	5
99	Identification of a predictive metabolic signature of response to immune checkpoint inhibitors in non-small cell lung cancer: METABO-ICI clinical study protocol. Respiratory Medicine and Research, 2021, 80, 100845.	0.6	3
100	New Insights in Pharmaceutical Analysis. Chimia, 2012, 66, 330.	0.6	2
101	Indirect quantitative structure-retention relationship for steroid identification: A chemometric challenge at "Chimiométrie 2016â€. Chemometrics and Intelligent Laboratory Systems, 2017, 160, 52-58.	3.5	2
102	Analysis of Metabolomics Data—A Chemometrics Perspective. , 2020, , 483-505.		2
103	Mass spectrometry metabolomic data handling for biomarker discovery. , 2020, , 369-388.		2
104	Efficiently handling highâ€dimensional data from multifactorial designs with unequal group sizes using Rebalanced ASCA (RASCA). Journal of Chemometrics, 2023, 37, .	1.3	2
105	Synergy at the ' <i>Ecole de Pharmacie Genève-Lausanne</i> ': Methodology Developments for the Treatment of Complex Metabolomic Datasets with Data Mining. Chimia, 2005, 59, 362-365.	0.6	1
106	Extracting Knowledge from MS Clinical Metabolomic Data: Processing and Analysis Strategies. Methods in Molecular Biology, 2018, 1730, 371-384.	0.9	1
107	Plant Metabolomics – Strategies for Biomarker Detection, Isolation, and Identification. Chimia, 2008, 62, 685.	0.6	0
108	Integration of Metabolomic Data From Multiple Analytical Platforms: Towards Extensive Coverage of the Metabolome. Comprehensive Analytical Chemistry, 2018, , 477-504.	1.3	0

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109	NMR- and UHPLC-MS correlation for identification of biomarkers from woods of Vitis Vinifera cultivar resistant to pathogens. Planta Medica, 2012, 78, .	1.3	0