Julien BOCCARD
January 4th 1978, Geneva
Swiss - Married (two children)

School of Pharmaceutical Sciences
1, rue Michel-Servet
1211 Geneva 4 - Switzerland
☎ +41 (0) 22 379 64 77
✉ julien.boccard@unige.ch

RESEARCH INTERESTS

- ★ Chemometrics
- ★ Multivariate analysis
- ★ Metabolomics
- ★ Data fusion
- ★ Bioinformatics
- ★ Machine learning

ACADEMIC QUALIFICATIONS

2009	**PhD in Sciences (with distinction).** "*Knowledge discovery in pharmaceutical sciences, from metabolomics to molecular modelling*". University of Geneva
2004	**Master of Advanced Studies in Bioinformatics.** Swiss Institute of Bioinformatics, University of Geneva
2002	**Master of Science in Biology.** University Medical Centre, University of Geneva
2000	**Bachelor of Science in Biology.** University of Geneva

PROFESSIONAL EXPERIENCE

since 2016	**Senior Research Associate.** School of Pharmaceutical Sciences, University of Geneva, University of Lausanne
2013-2015	**Senior Research and Teaching Assistant.** School of Pharmaceutical Sciences, University of Geneva, University of Lausanne
2012	**Post-doctoral Fellow.** "*Advanced chemometric analysis and integration of multiple Omics data: assessment of dioxin toxicity in human*". AgroParisTech, Paris (France)
2009-2011	**Research Associate.** Swiss Centre for Applied Human Toxicology (SCAHT), Geneva
2004-2009	**Research and Teaching Assistant.** School of Pharmaceutical Sciences, University of Geneva, University of Lausanne

LANGUAGES

French	Mother tongue
English	Professional working proficiency
German	Limited working proficiency

PROFESSIONAL ACTIVITIES

ACADEMIC ORGANIZATIONS

- Board member of the Mass Spectrometry: Applications to the Clinical Lab (MSACL) conference European Scientific Committee since 2018
- Board member of the Swiss Metabolomics Society (SMS) since 2017
- Board member of the Francophone Metabolomics and Fluxomics network (RFMF) since 2015
- Member of the Metabolomics Society, the Swiss Chemical Society (SCS), the French Statistical Society (SFdS), the Centre of Competence in Analytical Chemistry and Toxicology (ccCTA)

CONGRESS CO-ORGANISER

- Chimiométrie XVI, University of Geneva 19-21.01.2015
- 10èmes Journées Scientifiques du RFMF, Montpellier 30.05-02.06.2016
- Annual Meetings of the Swiss Metabolomics Society (since 2018)

GRANTS

Project funding. (Co-applicant, 2017) *"Steroidomics, an innovative metabolomic approach to extend the steroid profile monitoring in human".* Swiss National Science Foundation. 31003A_166658/1, 525'000 CHF.

Fellowship for advanced researcher. (Responsible applicant, 2012) *"Advanced chemometric analysis and integration of multiple Omics data: assessment of dioxin toxicity in human".* Swiss Foundation for Grants in Biology and Medicine. PASMP3_140064/1, 50'360 CHF.

BIBLIOMETRICS

5 PUBLICATION HIGHLIGHTS

- ★ **Gaining insights into metabolic networks using chemometrics and bioinformatics: chronic kidney disease as a clinical model.** J. Boccard, D. Schvartz, S. Codesido, M. Hanafi, Y. Gagnebin, B. Ponte, F. Jourdan, S. Rudaz. *Frontiers in Molecular Biosciences* (2021), 8, 682559. *[Research article]*
- ★ **Network principal component analysis: a versatile tool for the investigation of multigroup and multiblock datasets.** S. Codesido, M. Hanafi, Y. Gagnebin, V. González-Ruiz, S. Rudaz, J. Boccard. *Bioinformatics* (2020), btaa954. *[Research article]*
- ★ **Analysis of metabolomic data – A chemometrics perspective** in *Comprehensive Chemometrics (Second Edition),* J. Boccard, S. Rudaz. Elsevier (2020). *[Book chapter]*
- ★ **Exploring Omics data from designed experiments using Analysis of Variance Multiblock Orthogonal Partial Least Squares.** J. Boccard, S. Rudaz. *Analytica Chimica Acta* (2016), 920, 18-28. *[Research article]*
- ★ **A consensus OPLS-DA strategy for multiblock Omics data fusion.** J. Boccard, D.N. Rutledge. *Analytica Chimica Acta* (2013), 769, 30-39. *[Research article]*

Research articles: **88** Reviews/tutorials/perspective articles: **12**
Book chapters: **9** Invited short communications: **2**

h-index: 32 **i10-index: 66**
citations: >3'200 (Google Scholar, May 2021)

Oral communications: **23** Posters (as first author): **17**
External invited lectures: **21** (Denmark, Greece, France, Belgium, Switzerland)

PhD/Master thesis jury or committee: **19** (ONIRIS, AgroParisTech, Paris-Saclay University, Grenoble Alpes University, Clermont Auvergne University, University of Perpignan Via Domitia, Toulouse III - Paul Sabatier University, INRAe, University of Liège, University of Lausanne, University of Geneva)

PhD co-directions: **1** (University of Geneva)

PEER REVIEW DUTIES

Ad hoc reviewer for *Analytical Chemistry*, *Analytica Chimica Acta*, *Metabolomics*, *Bioinformatics*, *BMC Bioinformatics*, PLOS Computational Biology, *Chemometrics and Intelligent Laboratory Systems*, *Journal of Chemometrics, Journal of Chromatography A, Talanta, Analytical and Bioanalytical Chemistry*, *Journal of Pharmaceutical and Biomedical Analysis*, *Current Opinion in Toxicology*, *Forensic Science International*, *Metabolites, Molecules, Computer Methods and Programs in Biomedicine*, *Computational and Structural Biotechnology Journal, Phytochemistry, Chemosphere, Flavour and Fragrance Journal*, *Food Chemistry*, *Food Research International*, *LWT - Food Science and Technology*, *Journal of the Brazilian Chemical Society*, *Planta Medica, PeerJ*.

TEACHING

SCHOOL OF PHARMACEUTICAL SCIENCES (UNIVERSITY OF GENEVA, SWITZERLAND)

- Statistics & Pharmaceutical Methodology (Bachelor 2, since 2008, 24 h/y)
- Pharmaceutical Methodology (Bachelor 3, since 2010, 40 h/y)
- Multivariate Analysis (Doctoral program, since 2011, 16 h/y)
- Design of Experiments (Doctoral program, since 2011, 16 h/y)

FACULTY OF SCIENCES (UNIVERSITY OF GENEVA, SWITZERLAND)

- Biostatistics (MAS in Toxicology, since 2013, 32 h/2y)
- Metabolomics (MAS in Drug Discovery and Clinical Development, since 2017, 2 h/y)
- Elements of Proteomics & Metabolomics (Master, since 2017, 6 h/y)

SCHOOL OF CRIMINAL SCIENCES (UNIVERSITY OF LAUSANNE, SWITZERLAND)

- Design of Experiments (Master, since 2016, 2 h/y)

INTERUNIVERSITY DOCTORAL PROGRAM « STAROMICS » (UNIVERSITIES OF GENEVA, LAUSANNE, NEUCHÂTEL, FRIBOURG AND BERN, SWITZERLAND)

- Multivariate Analysis in Metabolomics (Doctoral program, since 2017, 3 h/y)

INTERUNIVERSITY DOCTORAL PROGRAM IN ORGANISMAL BIOLOGY (UNIVERSITIES OF GENEVA, LAUSANNE, NEUCHÂTEL, FRIBOURG AND BERN, SWITZERLAND)

- Metabolomics Data Analysis (Doctoral program, since 2014, 6 h/2y)

CENTRE OF COMPETENCE IN ANALYTICAL CHEMISTRY AND TOXICOLOGY (SWITZERLAND)

- Statistics in Toxicology (Continuing education, since 2011, 8 h/y)
- Multivariate Analysis (Continuing education, since 2015, 8 h/y)

SIGMA PLUS/DYNACENTRIX (PARIS, FRANCE)

- Multivariate Analysis of Omics Data (Training course, since 2011)

MASSIVE OPEN ONLINE COURSES

- CheMoocs (Chemometrics, since 2015)
- UseMetabo (Metabolomics, since 2018)

BARCAMPS / TRAINING WORKSHOPS

- ChemOmics (Chemometrics/Metabolomics, 2019 and 2021)

PEER-REVIEWED SCIENTIFIC ARTICLES

88. Gaining insights into metabolic networks using chemometrics and bioinformatics: chronic kidney disease as a clinical model. J. Boccard, D. Schvartz, S. Codesido, M. Hanafi, Y. Gagnebin, B. Ponte, F. Jourdan, S. Rudaz. *Frontiers in Molecular Biosciences* (2021), 8, 682559.

87. Neuroinflammatory response to TNFa and IL1β cytokines is accompanied by an increase of glycolysis in human astrocytes in vitro. D. Pamies, C. Sartori, D. Schvartz, V. González-Ruiz, L. Pellerin, C. Nunes, D. Tavel, V. Maillard, J. Boccard, S. Rudaz, J.-C. Sanchez, M.-G. Zurich. *International Journal of Molecular Sciences* (2021), 22(8), 4065.

86. Longitudinal evaluation of multiple biomarkers for the detection of testosterone gel administration in women with normal menstrual cycle. O. Salamin, R. Nicoli, T. Langer, J. Boccard, C. Schweizer Grundisch, C. Xu, S. Rudaz, N. Pitteloud, M. Saugy, T. Kuuranne. Accepted in *Drug Testing and Analysis* (in press).

85. Wipe sampling procedure optimization for the determination of 23 antineoplastic drugs used in hospital pharmacy. N. Guichard, J. Boccard, S. Rudaz, P. Bonnabry, S. Fleury-Souverain. *European Journal of Hospital Pharmacy* (2021), 28(2), 94-99.

84. Metabotypes of Pseudomonas aeruginosa correlate with antibiotic resistance, virulence and clinical outcome in cystic fibrosis chronic infections. O. Moyne, F. Castelli, D.J. Bicout, J. Boccard, B. Camara, B. Cournoyer, E. Faudry, S. Terrier, D. Hannani, S. Huot-Marchand, C. Leger, M. Maurin, T. Dung Ngo, C. Plazy, R.A. Quinn, I. Attree, F. Fenaille, B. Toussaint, A. Le Gouëllec. *Metabolites* (2021), 11(2), 63.

83. Evaluation of different tandem MS/MS acquisition modes to support metabolite annotation in human plasma using ultra high-performance liquid chromatography high-resolution mass spectrometry for untargeted metabolomics. J. Pezzatti, V. González-Ruiz, J. Boccard, D. Guillarme, S. Rudaz. *Metabolites* (2020), 10(11), 464.

82. Exploring blood alterations in chronic kidney disease and haemodialysis using metabolomics. Y. Gagnebin, D.A. Jaques, S. Rudaz, S. de Seigneux, J. Boccard, B. Ponte. *Scientific Reports* (2020), 10:19502.

81. Network principal component analysis: a versatile tool for the investigation of multigroup and multiblock datasets. S. Codesido, M. Hanafi, Y. Gagnebin, V. González-Ruiz, S. Rudaz, J. Boccard. *Bioinformatics* (2020), btaa954.

80. Inhibition of enteric methanogenesis in dairy cows induces changes in plasma metabolome highlighting metabolic shifts and potential markers of emission. B. Yanibada, U. Hohenester, M. Pétéra, C. Canlet, S. Durand, F. Jourdan, J. Boccard, C. Martin, M. Eugène, D. Morgavi, H. Boudra. *Scientific Reports* (2020), 10, 15591.

79. Insights on the structural and metabolic resistance of potato (Solanum tuberosum) cultivars to tuber black dot (Colletotrichum coccodes). J. Massana-Codina, S. Schnee, P.-M. Allard, A. Rutz, J. Boccard, E. Michellod, M. Cléroux, S. Schürch, K. Gindro, J.-L. Wolfender. *Frontiers in Plant Science* (2020), 11, 1287.

78. Multifactorial analysis of environmental metabolomic data in ecotoxicology: wild marine mussel exposed to WWTP effluent as a case study. T. Dumas, J. Boccard, E. Gomez, H. Fenet, F. Courant. *Metabolites* (2020), 10(7), 269.

77. Development and validation of an UHPLC-MS/MS method for extended serum steroid profiling in female populations. O. Salamin, F. Ponzetto, J. Boccard, S. Rudaz, M. Saugy, T. Kuuranne, R. Nicoli. *Bioanalysis* (2020), 12(11), 753-768.

76. Comprehensive examination of the mouse lung metabolome following *Mycobacterium tuberculosis* infection using a multiplatform mass spectrometry approach. M. Fernández-García, F. Rey-Stolle, J. Boccard, V. Reddy, A. García, B. Cumming, A. Steyn, S. Rudaz, C. Barbas. *Journal of Proteome Research* (2020), 19(5), 2053-2070.

75. Cultivar, site or harvest date: the Gordian knot of Wine Terroir. L. M. Schmidtke, G. Antalick, K. Šuklje, J W. Blackman, J. Boccard, A. Deloire. *Metabolomics* (2020), 16, 52.

74. Applicability of supercritical fluid chromatography – mass spectrometry to metabolomics. II-Assessment of a comprehensive library of metabolites and evaluation of biological matrices. G. L. Losacco, O. Ismail, J. Pezzatti, V. González-Ruiz, J. Boccard, S. Rudaz, J.-L. Veuthey, D. Guillarme. *Journal of Chromatography A* (2020), 1620, 461021.

73. Metabolomics approach reveals disruption of metabolic pathways in the marine bivalve *Mytilus galloprovincialis* exposed to a WWTP effluent extract. T. Dumas, B. Bonnefille, E. Gomez, J. Boccard, N. Ariza Castro, H. Fenet, F. Courant. *Science of the Total Environment* (2020), 712, 136551.

72. Profiling of anabolic androgenic steroids and selective androgen receptor modulators for interference with adrenal steroidogenesis. M. Patt, K. R. Beck, T. Di Marco, M.-C. Jäger, V. González-Ruiz, J. Boccard, S. Rudaz, C. van Koppen, M. Grill, A. Odermatt. *Biochemical Pharmacology* (2020), 172, 113781.

71. Supercritical Fluid Chromatography - Mass Spectrometry in routine anti-doping analyses: estimation of retention time variability under reproducible conditions. G. L. Losacco, E. Marconetto, R. Nicoli, T. Kuuranne, J. Boccard, S. Rudaz, J.-L. Veuthey, D. Guillarme. *Journal of Chromatography A* (2020), 1616, 460780.

70. Steroid profile analysis by LC-HR-MS in human seminal fluid. E. Olesti, A. Garcia, R. Rahban, M. Rossier, J. Boccard, S. Nef, V. González-Ruiz, S. Rudaz. *Journal of Chromatography B* (2020), 1136, 121929.

69. Combining the advantages of multilevel and orthogonal partial least squares data analysis for longitudinal metabolomics: application to kidney transplantation. Y. Gagnebin, J. Pezzatti, P. Lescuyer, J. Boccard, B. Ponte, S. Rudaz. *Analytica Chimica Acta* (2020), 109, 26-38.

68. Choosing an optimal sample preparation in *Caulobacter crescentus* for untargeted metabolomics approaches. J. Pezzatti, M. Bergé, J. Boccard, S. Codesido, Y. Gagnebin, P. H. Viollier, V. González-Ruiz, S. Rudaz. *Metabolites* (2019), 9(10), 193.

67. Processing of NMR and MS metabolomics data using chemometrics methods: a global tool for fungi biotransformation reactions monitoring. C. Palaric, S. Pilard, J.-X. Fontaine, J. Boccard, D. Mathiron, S. Rigaud, D. Cailleu, F. Mesnard, Y. Gut, T. Renaud, A. Petit, J.-Y. Beaumal, R. Molinié. *Metabolomics* (2019), 15, 107.

66. Protein pathway analysis to study development-dependent effects of acute and repeated Trimethyltin (TMT) treatments in 3D rat brain cell cultures. D. Schvartz, V. González-Ruiz, N. Walter, P. Antinori, F. Jeanneret, D. Tonoli, J. Boccard, M.-G. Zurich, S. Rudaz, F. Tschudi-Monnet, J. Sandström, J.-C. Sanchez. *Toxicology in Vitro* (2019), 60, 281-292.

65. Steroidomics for highlighting novel serum biomarkers of testosterone doping. F. Ponzetto, J. Boccard, R. Nicoli, T. Kuuranne, M. Saugy, S. Rudaz. *Bioanalysis* (2019), 11(12), 1171-1187.

64. DynaStI: A dynamic retention time database for steroidomics. S. Codesido, G. M. Randazzo, F. Lehmann, V. González-Ruiz, A. García, I. Xenarios, R. Liechti, A. Bridge, J. Boccard, S. Rudaz. *Metabolites* (2019), 9(5), 85.

63. An integrative multi-omics workflow to address multifactorial toxicology experiments. V. González-Ruiz, D. Schvartz, J. Sandström, J. Pezzatti, F. Jeanneret, D. Tonoli, J. Boccard, F. Monnet-Tschudi, J.-C. Sanchez, S. Rudaz. *Metabolites* (2019), 9(4), 79.

62. In vitro models to study insulin and glucocorticoids modulation of Trimethyltin (TMT)-induced neuroinflammation and neurodegeneration, and in vivo validation in db/db mice. J. Sandström, D. Kratschmar, A. Broyer, O. Poirot, P. Marbet, B. Chantong, F. Zufferey, T. Dos Santos, J. Boccard, R. Chrast, A. Odermatt, F. Monnet-Tschudi. *Archives of Toxicology* (2019), 93(6), 1649-1664.

61. Toward a better understanding of chronic kidney disease with complementary chromatographic methods hyphenated with mass spectrometry for improved polar metabolome coverage. Y. Gagnebin, J. Pezzatti, P. Lescuyer, J. Boccard, B. Ponte, S. Rudaz. *Journal of Chromatography B* (2019), 1116, 9-18.

60. Chemical composition and anti-inflammatory activity of the decoction from leaves of a cultivated specimen of *Myracrodruon urundeuva*. N. C. Aquino, E. F. Queiroz, L. Marcourt, L. B. N. Freitas, E. V. O. Araújo, L. K. A. M. Leal, A. M. E. Bezerra, J. Boccard, J.-L. Wolfender, E. R. Silveira. *Journal of the Brazilian Chemical Society* (2019), 30(8), 1616-1623.

59. A scoring approach for multi-platform acquisition in metabolomics. J. Pezzatti, V. González-Ruiz, S. Codesido, Y. Gagnebin, A. Joshi, D. Guillarme, J. Schappler, D. Picard, J. Boccard, S. Rudaz. *Journal of Chromatography A* (2019), 1592, 47-54.

58. Removal of batch effects using stratified subsampling of metabolomic data for *in vitro* endocrine disruptors screening. J. Boccard, D. Tonoli, P. Strajhar, F. Jeanneret, A. Odermatt, S. Rudaz. *Talanta* (2019), 195, 77-86.

57. 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. F. Zufferey, R. Rahban, A. Garcia, Y. Gagnebin, J. Boccard, D. Tonoli, F. Jeanneret, E. Stettler, A. Senn, S. Nef, S. Rudaz, M. Rossier. *Clinical Biochemistry* (2018), 62, 39-46.

56. Dynamics of metabolite induction in fungal co-cultures by metabolomics at both volatile and non-volatile levels. A. Azzollini, L. Boggia, J. Boccard, B. Sgorbini, N. Lecoultre, P.-M. Allard, P. Rubiolo, S. Rudaz, K. Gindro, C. Bicchi, J.-L. Wolfender. *Frontiers in Microbiology* (2018), 9, 72.

55. 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. V. González-Ruiz, J. Pezzatti, A. Roux, L. Stoppini, J. Boccard, S. Rudaz. *Journal of Chromatography A* (2017), 1527, 53-60.

54. Enhanced metabolite annotation via dynamic retention time prediction: steroidogenesis alterations as a case study. G. M. Randazzo, D. Tonoli, P. Strajhar, I. Xenarios, A. Odermatt, J. Boccard, S. Rudaz. *Journal of Chromatography B* (2017), 1071, 11-18.

53. Optimized selection of liquid chromatography conditions for wide range analysis of natural compounds. A. Périat, D. Guillarme, J.-L. Veuthey, J. Boccard, S. Moco, D. Barron, A. Grand-Guillaume Perrenoud. *Journal of Chromatography A* (2017), 1504, 91-104.

52. High resolution mass spectrometry as an alternative detection method to tandem mass spectrometry for the analysis of endogenous steroids in serum. F. Ponzetto, J. Boccard, N. Baume, T. Kuuranne, S. Rudaz, M. Saugy, R. Nicoli. *Journal of Chromatography B* (2017), 1052, 34-42.

51. Steroid profiling in H295R cells to identify chemicals potentially disrupting the production of adrenal steroids. P. Strajhar, D. Tonoli, F. Jeanneret, R. M. Imhof, V. Malagnino, M. Patt, D. V. Kratschmar, J. Boccard, S. Rudaz, A. Odermatt. *Toxicology* (2017), 381, 51–63.

50. Metabolomic analysis of urine samples by UHPLC-QTOF-MS: impact of normalization strategies. Y. Gagnebin, D. Tonoli, P. Lescuyer, B. Ponte, S. de Seigneux, P.-Y. Martin, J. Schappler, J. Boccard, S. Rudaz. *Analytica Chimica Acta* (2017), 955, 27-35.

49. Targeted metabolomics shows plasticity in the evolution of signaling lipids and uncovers old and new endocannabinoids in the plant kingdom. M. S. Gachet, A. Schubert, S. Calarco, J. Boccard, J. Gertsch. *Scientific Reports* (2017), 7, 41177.

48. Indirect Quantitative Structure-Retention Relationship for Steroid Identification: A chemometric challenge at "Chimiométrie 2016". G. M. Randazzo, E. Vigneau, P. Courcoux, C. Harrouet, Y. Lijour, P. Dardenne, J. Boccard, S. Rudaz. *Chemometrics and Intelligent Laboratory Systems* (2017), 160, 52-58.

47. Structured plant metabolomics for the simultaneous exploration of multiple factors. N. Vasilev, J. Boccard, G. Lang, U. Grömping, R. Fischer, S. Goepfert, S. Rudaz, S. Schillberg. *Scientific Reports* (2016), 6, 37390.

46. A Standardized LCxLC-ELSD Fractionation Procedure for the Identification of Minor Bioactives via the Enzymatic Screening of Natural Extracts. P. Coulerie, Y. Ratinaud, S. Moco, L. Merminod, M. Naranjo Pinta, J. Boccard, L. Bultot, M. Deak, K. Sakamoto, E. Queiroz, J.-L. Wolfender, D. Barron. *Journal of Natural Products* (2016), 79(11), 2856–2864.

45. High throughput identification of monoclonal antibodies after compounding by UV spectroscopy coupled to chemometrics analysis. E. Jaccoulet, J. Boccard, M. Taverna, A. Santos Azevedos, S. Rudaz, C. Smadja. *Analytical and Bioanalytical Chemistry* (2016), 408, 5915–5924.

44. Ultra-high Performance Supercritical Fluid Chromatography coupled with quadrupole-time-of-flight mass spectrometry as a performing tool for bioactive analysis. A. Grand-Guillaume Perrenoud, D. Guillarme, J. Boccard, J.-L. Veuthey, D. Barron, S. Moco. *Journal of Chromatography A* (2016), 1450, 101–111.

43. Exploring Omics data from designed experiments using Analysis of Variance Multiblock Orthogonal Partial Least Squares. J. Boccard, S. Rudaz. *Analytica Chimica Acta* (2016), 920, 18-28.

42. Prediction of retention time in reversed-phase liquid chromatography as a tool for steroid identification. G. M. Randazzo, D. Tonoli, S. Hambye, D. Guillarme, F. Jeanneret, A. Nurisso, L. Goracci, J. Boccard, S. Rudaz. *Analytica Chimica Acta* (2016), 916, 8-16.

41. Statistical correlations between HPLC activity-based profiling results and NMR/MS microfractions data to deconvolute bioactive compounds in mixture. S. Bertrand, A. Azzollini, A. Nievergelt, J. Boccard, S. Rudaz, M. Cuendet, J.-L. Wolfender. *Molecules* (2016), 21(3), 259.

40. Longitudinal monitoring of endogenous steroids in human serum by UHPLC-MS/MS as a tool to detect testosterone abuse in sport. F. Ponzetto, F. Mehl, J. Boccard, N. Baume, S. Rudaz, M. Saugy, R. Nicoli. *Analytical and Bioanalytical Chemistry* (2016), 408(3), 705-719.

39. Systematic evaluation of matrix effects in hydrophilic interaction chromatography versus reversed phase liquid chromatography coupled to mass spectrometry. A. Périat, I. Kohler, A. Thomas, R. Nicoli, J. Boccard, J.-L. Veuthey, J. Schappler, D. Guillarme. *Journal of Chromatography A* (2016), 1439, 42–53.

38. Evaluation and identification of dioxin exposure biomarkers in human urine by high-resolution metabolomics, multivariate analysis and in vitro synthesis. F. Jeanneret, D. Tonoli, D. Hochstrasser, J.-H. Saurat, O. Sorg, J. Boccard, S. Rudaz. *Toxicology Letters* (2016), 240(1), 22–31.

37. Rumen microbial communities influence metabolic phenotypes in lambs. D. Morgavi, E. Rathahao-Paris, M. Popova, J. Boccard, K. Fog Nielsen, H. Boudra. *Frontiers in Microbiology* (2015), 6, 1060.

36. 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. D. Tonoli, C. Fürstenberger, J. Boccard, D. Hochstrasser, F. Jeanneret, A. Odermatt, S. Rudaz. *Chemical Research in Toxicology* (2015), 28(5), 955−966.

35. Assessing susceptibility to epilepsy in three rat strains using brain metabolic profiling based on HRMAS NMR spectroscopy and chemometrics. F. Fauvelle, J. Boccard, F. Cavarec, A. Depaulis, C. Deransart. *Journal of Proteome Research* (2015), 14(5), 2177−2189.

34. Integrating metabolomic data from multiple analytical platforms for a comprehensive characterisation of lemon essential oils. F. Mehl, G. Marti, P. Merle, E. Delort, L. Baroux, H. Sommer, J.-L. Wolfender, S. Rudaz, J. Boccard. *Flavour and Fragrance Journal* (2015), 30, 131–138.

33. Multi-way PLS regression: Monotony convergence of tri-linear PLS2 and optimality of parameters. M. Hanafi, S. Ouertani, G. Mazerolles, J. Boccard, S. Rudaz. *Computational Statistics and Data Analysis* (2015), 83, 129–139.

32. Retention time prediction for dereplication of natural products ($C_xH_yO_z$) in LC-MS metabolite profiling. P.J. Eugster, J. Boccard, B. Debrus, L. Bréant, J.-L. Wolfender, S. Martel, P.-A. Carrupt. *Phytochemistry* (2014), 108, 196-207.

31. Untargeted profiling of urinary steroid metabolites after testosterone ingestion: opening new perspectives for anti-doping testing. J. Boccard, F. Badoud, N. Jan, R. Nicoli, C. Schweizer, F. Pralong, J.-L. Veuthey, N. Baume, S. Rudaz, M. Saugy. *Bioanalysis* (2014), 6(19), 2523-2536.

30. Quantitative monitoring of tamoxifen in human plasma extended to forty metabolites using LC-HR-MS: New investigation capabilities for clinical pharmacology. E. Dahmane, J. Boccard, C. Csajka, S. Rudaz, L. Décosterd, E. Genin, B. Duretz, M. Bromirski, K. Zaman, B. Testa, B. Rochat. *Analytical and Bioanalytical Chemistry* (2014), 406(11), 2627-2640.

29. Multi-way PLS for discrimination: Compact form equivalent to the tri-linear PLS2 procedure and its monotony convergence. S. Ouertani, M. Hanafi, G. Mazerolles, J. Boccard, S. Rudaz. *Chemometrics and Intelligent Laboratory Systems* (2014), 133, 25-32.

28. Iterative weighting of multiblock data in the Orthogonal Partial Least Squares framework. J. Boccard, D.N. Rutledge. *Analytica Chimica Acta* (2014), 813, 25–34.

27. Human urinary biomarkers of dioxin exposure: analysis by metabolomics and biologically-driven data dimensionality reduction. F. Jeanneret, J. Boccard, F. Badoud, O. Sorg, D. Pelclova, S. Vlckova, D.N. Rutledge, C. F. Samer, D. Hochstrasser, J.-H. Saurat, S. Rudaz. *Toxicology Letters* (2014), 230, 234-243.

26. Comprehensive profiling and marker identification in non-volatile citrus oil residues by mass spectrometry and nuclear magnetic resonance. G. Marti, J. Boccard, F. Mehl, B. Debrus, L. Marcourt, P. Merle, E. Delort, L. Baroux, H. Sommer, S. Rudaz, J.-L. Wolfender. *Food Chemistry* (2014), 150, 235-245.

25. Differentiation of lemon essential oil based on volatile and non-volatile fractions with various analytical techniques: a metabolomic approach. F. Mehl, G. Marti, J. Boccard, B. Debrus, P. Merle, E. Delort, L. Baroux, V. Raymo, M.I. Velazco, H. Sommer, J.-L. Wolfender, S. Rudaz. *Food Chemistry* (2014), 143, 325-335.

24. Systematic comparison of sensitivity between HILIC-MS and RPLC-MS using columns packed with sub-2 µm particles. A. Périat, J. Boccard, J.-L. Veuthey, S. Rudaz, D. Guillarme. *Journal of Chromatography A* (2013), 1312, 49-57.

23. Différentiation d'huile essentielle de citron basée sur l'analyse des fractions volatile et non-volatile par plusieurs techniques analytiques : une approche métabolomique. F. Mehl, G. Marti, J. Boccard, B. Debrus, P. Merle, E. Delort, L. Baroux, V. Raymo, M. I. Velazco, H. Sommer, J.-L. Wolfender, S. Rudaz. *Spectra Analyse* (2013), 294, 48-58.

22. 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. F. Badoud, J. Boccard, C. Schweizer, F. Pralong, M. Saugy, N. Baume. *The Journal of Steroid Biochemistry and Molecular Biology* (2013), 138, 222-235.

21. A consensus OPLS-DA strategy for multiblock Omics data fusion. J. Boccard, D.N. Rutledge. *Analytica Chimica Acta* (2013), 769, 30-39.

20. Metabolomics reveals herbivore-induced metabolites of resistance and susceptibility in maize leaves and roots. G. Marti, M. Erb, J. Boccard, G. Glauser, G.D. Doyen, N. Villard, C.A.M. Robert, T.C.J. Turlings, S. Rudaz, J.-L. Wolfender. *Plant, Cell and Environment* (2013), 36(3), 621-639.

19. Analysis of basic compounds by supercritical fluid chromatography: Attempts to improve peak shape and maintain mass spectrometry compatibility. A. Grand-Guillaume Perrenoud, J. Boccard, J.-L. Veuthey, D. Guillarme. *Journal of Chromatography A* (2012), 1262, 205-213.

18. Analyse métabolomique dans l'urine par UHPLC-QTOF-MS^E: profilage des stéroïdes appliqué au dépistage anti-dopage. J. Boccard, F. Badoud, E. Grata, S.S. Ouertani, M. Hanafi, G. Mazerolles, P. Lantéri, J.-L. Veuthey, M. Saugy, S. Rudaz. *Spectra Analyse* (2012), 41(284), 48-54.

17. Method development for pharmaceutics: Some solutions for tuning selectivity in reversed phase and hydrophilic interaction liquid chromatography. J. Ruta, Josephine; J. Boccard, D. Cabooter, S. Rudaz, G. Desmet, J.-L. Veuthey, D. Guillarme. *Journal of Pharmaceutical and Biomedical Analysis* (2012), 63, 95-105.

16. A steroidomic approach for biomarkers discovery in doping control. J. Boccard, F. Badoud, E. Grata, S.S. Ouertani, M. Hanafi, G. Mazerolles, P. Lantéri, J.-L. Veuthey, M. Saugy, S. Rudaz. *Forensic Science International*. (2011), 213(1-3), 85-94.

15. Quantification of glucuronidated and sulfated steroids in human urine by ultra-high pressure liquid chromatography quadrupole time-of-flight mass spectrometry. F. Badoud, E. Grata, J. Boccard, D. Guillarme, J.-L. Veuthey, S. Rudaz, M. Saugy. *Analytical and Bioanalytical Chemistry* (2011), 400(2), 503-516.

14. Analysis of experimental design with multivariate response: A contribution using multiblock techniques. G. Mazerolles, J. Boccard, M. Hanafi, S. Rudaz. *Chemometrics and Intelligent Laboratory Systems* (2011), 106(1), 65-72.

13. Phenotypic and molecular characterization of proliferating and differentiated GnRH-expressing GnV-3cells. V. Mansuy, S. Geller, J.-P. Rey, C. Campagne, J. Boccard, P. Poulain, V. Prevot, F. Pralong. *Molecular and Cellular Endocrinology* (2011), 332(1-2), 97-105.

12. Standard machine learning algorithms applied to UPLC-TOF/MS metabolic fingerprinting for the discovery of wound biomarkers in *Arabidopsis thaliana*. J. Boccard, A. Kalousis, M. Hilario, P. Lantéri, M. Hanafi, G. Mazerolles, J.-L. Wolfender, P.-A. Carrupt, S. Rudaz. *Chemometrics and Intelligent Laboratory Systems* (2010), 104(1), 20-27.

11. IEF pattern classification-derived criteria for the identification of epoetin-δ in urine. S. Lamon, J. Boccard, P.-E. Sottas, N. Glatz, G. Wuerzner, N. Robinson, M. Saugy. *Electrophoresis* (2010), 31(12), 1918-1924.

10. Mass spectrometry-based metabolomics oriented by correlation analysis for wound-induced molecule discovery: identification of a novel jasmonate glucoside. G. Glauser, J. Boccard, S. Rudaz, J.-L. Wolfender. *Phytochemical Analysis* (2010), 21(1), 95-101.

9. Breast cancer resistance protein (BCRP/ABCG2): New inhibitors and QSAR studies by a 3D linear solvation energy approach. E. Nicolle, J. Boccard, D. Guilet, M.-G. Dijoux-Franca, F. Zelefac, S. Macalou, J. Grosselin, J. Schmidt, P.-A. Carrupt, A. Di Pietro, A. Boumendjel. *European Journal of Pharmaceutical Sciences* (2009), 38(1), 39-46.

8. Metabolite profiling of plant extracts by ultra-high-pressure liquid chromatography at elevated temperature coupled to time-of-flight mass spectrometry. E. Grata, D. Guillarme, G. Glauser, J. Boccard, P.-A. Carrupt, J.-L. Veuthey, S. Rudaz, J.-L. Wolfender. *Journal of Chromatography A* (2009), 1216(30), 5660-5668.

7. A 3D linear solvation energy model to quantify the affinity of flavonoid derivatives toward P-glycoprotein. J. Boccard, F. Bajot, A. Di Pietro, S. Rudaz, A. Boumendjel, E. Nicolle, P.-A. Carrupt. *European Journal of Pharmaceutical Sciences* (2009), 36(2-3), 254-264.

6. UPLC-TOF-MS for plant metabolomics: A sequential approach for wound marker analysis in *Arabidopsis thaliana*. E. Grata, J. Boccard, D. Guillarme, G. Glauser, P.-A. Carrupt, E.E. Farmer, J.-L. Wolfender, S. Rudaz. *Journal of Chromatography B* (2008), 871(2), 261-270.

5. Antimitotic and antiproliferative activities of chalcones: forward structure-activity relationship. A. Boumendjel, J. Boccard, P.-A. Carrupt, E. Nicolle, M. Blanc, A. Geze, L. Choisnard, D. Wouessidjewe, E.-L. Matera, C. Dumontet. *Journal of Medicinal Chemistry* (2008), 51(7), 2307-2310.

4. Optimized liquid chromatography-mass spectrometry approach for the isolation of minor stress biomarkers in plant extracts and their identification by capillary nuclear magnetic resonance. G. Glauser, D. Guillarme, E. Grata, J. Boccard, A. Thiocone, P.-A. Carrupt, J.-L. Veuthey, S. Rudaz, J.-L. Wolfender. *Journal of Chromatography A* (2008), 1180(1-2), 90-98.

3. Development of a two-step screening ESI-TOF-MS method for rapid determination of significant stress-induced metabolome modifications in plant leaf extracts: the wound response in *Arabidopsis thaliana* as a case study. E. Grata, J. Boccard, G. Glauser, P.-A. Carrupt, E.E. Farmer, J.-L. Wolfender, S. Rudaz. *Journal of Separation Science* (2007), 30(14), 2268-2278.

2. Multivariate data analysis of rapid LC-TOF/MS experiments from *Arabidopsis thaliana* stressed by wounding. J. Boccard, E. Grata, A. Thiocone, J.-Y. Gauvrit, P. Lanteri, P.-A. Carrupt, J.-L. Wolfender, S. Rudaz. *Chemometrics and Intelligent Laboratory Systems* (2007), 86(2), 189-197.

1. CD40-CD40 ligand disruption does not prevent hyperoxia-induced injury. C. Barazzone Argiroffo, Y.R. Donati, J. Boccard, A.F. Rochat, C. Vesin, C.-D. Kan, P.-F. Piguet. *American Journal of Pathology* (2002), 160(1), 67-71.

PEER-REVIEWED SCIENTIFIC REVIEWS, TUTORIALS & PERSPECTIVE ARTICLES

12. Approaches in metabolomics for regulatory toxicology applications. E. Olesti, V. González-Ruiz, M.F. Wilks, J. Boccard, S. Rudaz. *Analyst* (2021), 146, 1820-1834.

11. From a single steroid to the steroidome: trends and analytical challenges. E. Olesti, J. Boccard, G. Visconti, V. González-Ruiz, S. Rudaz. *Journal of Steroid Biochemistry and Molecular Biology* (2021), 206:105797.

10. Implementation of liquid chromatography-high resolution mass spectrometry methods for untargeted metabolomic analyses of biological samples: a tutorial. J. Pezzatti, J. Boccard, S. Codesido, Y. Gagnebin, A. Joshi, D. Picard, V. González-Ruiz, S. Rudaz. *Analytica Chimica Acta* (2020), 1105, 28-44.

9. Metabolomics in chronic kidney disease: Strategies for extended metabolome coverage. Y. Gagnebin, J. Boccard, B. Ponte, S. Rudaz. *Journal of Pharmaceutical and Biomedical Analysis* (2018), 161, 313-325.

8. Evaluation of steroidomics by liquid chromatography hyphenated to mass spectrometry as a powerful analytical strategy for measuring human steroid perturbations. F. Jeanneret, D. Tonoli, M. Rossier, M. Saugy, J. Boccard, S. Rudaz. *Journal of Chromatography A* (2016), 1430, 97–112.

7. Harnessing the complexity of metabolomic data with chemometrics. J. Boccard, S. Rudaz. *Journal of Chemometrics* (2014), 28(1), 1-9.

6. New Insights in Pharmaceutical Analysis. D. Guillarme, J. Schappler, J. Boccard, J.-L. Veuthey, S. Rudaz. *Chimia* (2012), 66, 330-334.

5. Analytical aspects in doping control: Challenges and perspectives. F. Badoud, D. Guillarme, J. Boccard, E. Grata, M. Saugy, S. Rudaz, J.-L. Veuthey. *Forensic Science International*. (2011), 213(1-3), 49-61.

4. Knowledge discovery in metabolomics: an overview of MS data handling. J. Boccard, J.-L. Veuthey, S. Rudaz. *Journal of Separation Science* (2010), 33(3), 290-304.

3. MS-based plant metabolomic approaches for biomarker discovery. J.-L. Wolfender, G. Glauser, J. Boccard, S. Rudaz. *Natural Product Communications* (2009), 4(10), 1417-1430.

2. Plant metabolomics - strategies for biomarker detection, isolation, and identification. E. Grata, J. Boccard, G. Glauser, D. Guillarme, P.-A. Carrupt, J.-L. Wolfender, S. Rudaz. *Chimia* (2008), 62(7-8), 685.

1. Synergy at the 'Ecole de Pharmacie Geneve-Lausanne': Methodology developments for the treatment of complex metabolomic datasets with data mining. A. Thiocone, E. Grata, J. Boccard, P.-A. Carrupt, S. Rudaz, J.-L. Wolfender. *Chimia* (2005), 59(6), 362-365.

INVITED SHORT COMMUNICATIONS

2. Longitudinal Monitoring of Endogenous Blood Steroids as a Tool to Detect Testosterone Abuse in Sport. F. Ponzetto, J. Boccard, N. Baume, S. Rudaz, M. Saugy, R. Nicoli, *Chimia* (2016), 70(3), 208.

1. Plant Metabolomics – Strategies for Biomarker Detection, Isolation and Identification. E. Grata, J. Boccard, G. Glauser, D. Guillarme, P.-A. Carrupt, J.-L. Wolfender, S. Rudaz, *Chimia* (2008), 62(7/8), 685.

BOOK CHAPTERS

9. Analysis of metabolomic data – A chemometrics perspective in *Comprehensive Chemometrics (Second Edition),* J. Boccard, S. Rudaz. Elsevier (2020).

8. Mass Spectrometry Metabolomic Data Handling For Biomarker Discovery in *Proteomic and Metabolomic Approaches to Biomarker Discovery (Second Edition)*, J. Boccard, V. González-Ruiz, S. Codesido, S. Rudaz. Academic Press (2020).

7. Integration of metabolomic data from multiple analytical platforms: toward extensive coverage of the metabolome in *Data Analysis for Omic Sciences: Methods and Applications,* J. Boccard, S. Rudaz. Elsevier (2018).

6. UHPLC-HRMS analysis for steroid profiling in serum (steroidomics) in *Metabolic Profiling: Methods and Protocols,* F. Ponzetto, J. Boccard, R. Nicoli, T. Kuuranne, M. Saugy, S. Rudaz. Springer (2018).

5. Extracting knowledge from MS clinical metabolomic data: Processing and analysis strategies in *Clinical Metabolomics: Methods and Protocols,* J. Boccard, S. Rudaz. Springer (2018).

4. Methods for Doping Detection in *Sports Endocrinology,* F. Ponzetto, S. Giraud, N. Leuenberger, J. Boccard, R. Nicoli, N. Baume, S. Rudaz, M. Saugy. Karger (2016).

3. From raw signals to identified metabolites: recent tools for enhancing LC-MS untargeted metabolomic data processing in *Metabolomic Data Processing and Analysis,* D. Tonoli, F. Jeanneret, J. Boccard, S. Rudaz. Future Science (2015).

2. Mass Spectrometry Metabolomic Data Handling For Biomarker Discovery in *Proteomic and Metabolomic Approaches to Biomarker Discovery*, J. Boccard, S. Rudaz. Academic Press (2013).

1. Metabolomics: Application in plant sciences in *Metabolomics In Practice: Successful Strategies to Generate and Analyze Metabolic Data*, G. Glauser, J. Boccard, J.-L. Wolfender, S. Rudaz. Wiley-VCH (2013).

ORAL COMMUNICATIONS

23. Facing the data deluge: a practical survival guide. *33rd Seminar in Pharmaceutical Sciences*, September 2019, Zermatt (Switzerland).

22. Facing the data deluge: a practical guide to biomarker discovery. *CITB seminar series*, June 2019, Geneva (Switzerland).

21. Stratified subsampling for effective removal of batch effects in metabolomics: application to endocrine disruptors screening. *Chimiométrie XX*, February 2019, Montpellier (France).

20. Steroidomic profiling in an adrenal cell model, *6th SCAHT Science Advisory Board Meeting*, August 2018, Olten (Switzerland).

19. Exploring human urinary biomarkers of dioxin exposure using metabolomics and biologically-driven data dimensionality reduction. *3rd Meeting of the Swiss Metabolomics Society*, November 2017, Bern (Switzerland).

18. Toward a better understanding of neuroinflammation using proteomic and metabolomic data integration. *SCAHT Retreat*, August 2017, Neuchâtel (Switzerland).

17. Multiblock data integration and its application to plant metabolomics. *French Flax Research Network,* May 2017, Amiens (France).

16. Metabolomic profiles alterations induced by neuroinflammatory conditions, *5th SCAHT Science Advisory Board Meeting*, July 2016, Bern (Switzerland).

15. Exploring metabolomic data from designed experiments using ANOVA-Multiblock Orthogonal Partial Least Squares. *12th Annual Conference of the Metabolomics Society*, June 2016, Dublin (Ireland).

14. ANOVA-Multiblock Orthogonal Partial Least Squares (AMOPLS) for exploring metabolomic data from designed experiments. *Chimiométrie XVII*, January 2016, Namur (Belgium).

13. Analysis of metabolomic data from designed experiments using ANOVA Multiblock Orthogonal Partial Least Squares. *9èmes Journées Scientifiques du Réseau Francophone de Métabolomique et Fluxomique*, June 2015, Lille (France).

12. A consensus OPLS-DA strategy for multiblock data fusion: Application to plant metabolomics. *8èmes Journées Scientifiques du Réseau Francophone de Métabolomique et Fluxomique*, May 2014, Lyon (France).

11. Extension du profilage urinaire des stéroïdes par une approche stéroïdomique pour le dépistage anti-dopage. *7èmes Journées Scientifiques du Réseau Francophone de Métabolomique et Fluxomique*, June 2013, Amiens (France).

10. Pondération itérative de tableaux multiples dans le cadre de la modélisation OPLS multiblocs. *Chimiométrie XIV*, December 2012, Lille (France).

9. A multiblock OPLS-DA strategy for Omics data fusion. *Séminaire d'inauguration du DIM Analytics.* June 2012. Saclay (France).

8. A steroidomic strategy for profile monitoring in doping control analysis. *Annual Meeting of the Swiss Group for Mass Spectrometry,* October 2011, Beatenberg (Switzerland).

7. A metabolomic approach to extend the steroid profile monitoring for doping control analysis. *36th International Symposium on High-Performance Liquid Phase Separations and Related Techniques*, June 2011, Budapest (Hungary).

6. Machine learning applied to UPLC-TOF/MS metabolic fingerprinting for the discovery of wound biomarkers in *Arabidopsis thaliana*. *Chimiométrie XI*, December 2009, Paris (France).

5. Analyses métabolomiques en phytochimie. with J.-L. Wolfender, *Journées Scientifiques du ccCTA*, September 2008, Les Diablerets (Suisse).

4. Data mining of UPLC-TOF/MS metabolic fingerprints for the detection of wound biomarkers in *Arabidopsis thaliana*. *PhD Day*, June 2008, Archamps (France).

3. Analyse solvatochromique 3D des forces d'interactions moléculaires dirigeant la liaison de dérivés de flavonoïdes à la glycoprotéine P. *Chimiométrie IX*, November 2007, Lyon (France).

2. Analyse multivariée de données obtenues par gradient rapide LCTOF-MS dans le cadre d'une étude métabolomique chez *A. thaliana*. *Chimiométrie VII*, December 2005, Lille (France).

1. Statistical comparison of LC-MS ion maps in metabolomic studies. *Fall Meeting of the Swiss Chemical Society*, October 2004, Zürich (Suisse).

EXTERNAL INVITED LECTURES

21. Approches méthodologiques en métabolomique: de l'acquisition à l'analyse de données. Workshop. e*Chimiométrie*, January 2021, online.

20. Aspects méthodologiques pour l'acquisition et le traitement de données métabolomiques. Workshop. *Chimiométrie XXI*, January 2020, Liège (Belgium).

19. Advanced approaches for the analysis of metabolomics data: From experimental design to knowledge discovery. *RFMF-Metabomeeting*, January 2020, Toulouse (France).

18. On the trail of biomarkers: Principles and chemometric approaches for the analysis of metabolomic data. *Seminar series*, July 2019, Laboratoire d'Etude des Résidus et Contaminants dans les Aliments (LABERCA), ONIRIS, Nantes (France).

17. Data integration in metabolomics: food for thought in bioinformatics and chemometrics. *Data Integration Workshop, 12èmes Journées Scientifiques du Réseau Francophone de Métabolomique et Fluxomique,* May 2019, Clermont-Ferrand (France).

16. Current challenges in metabolomics: From experimental design to knowledge discovery, *MetaToul Seminars*, May 2019, Toulouse (France).

15. Chemometrics and bioinformatics for metabolomics, *Bioinformatic Network Workshop*, April 2019, Geneva (Switzerland).

14. L'Analyse Multivariée des Données Expérimentales. Tutorial. *13ème Congrès de l'Association Francophone des Sciences Séparatives*, March 2019, Paris (France).

13. Multivariate analysis of metabolomic data. *Metabolomics for life and health scientists*, December 2018, Lausanne (Switzerland).

12. Data Structures and Advanced Chemometric Tools in Metabolomics. *Workflow4Experimenters workshop, Pasteur Institute,* October 2018, Paris (France).

11. Data Structures and Chemometric Strategies in Metabolomics. *BIOPI seminars, University of Picardy Jules Verne,* June 2018, Amiens (France).

10. Chemometric approaches for Meta²bolomics. *Meta-metabolomics Workshop, 11èmes Journées Scientifiques du Réseau Francophone de Métabolomique et Fluxomique,* May 2018, Liège (Belgium).

9. A multiblock approach for the integration of multiple data sources in metabolomics. *Club Lyonnais de Chromatographie, Forum Labo,* March 2018, Lyon (France).

8. Multivariate analysis of metabolomic data. *Metabolomics: from data to publication*, June 2017, Lausanne (Switzerland).

7. Sur la piste des biomarqueurs : Traitement des données métabolomiques obtenues par chromatographie liquide couplée à la spectrométrie de masse. *Société des Experts Chimistes de France*, June 2017, Solaize (France).

6. Advanced chemometric methods for MS-based metabolomics. *Métabolomique: Outils et méthodologie,* April 2016, Clermont-Ferrand (France).

5. Chemometric approaches for the fusion of multiple data sources in metabolomics. *Applied Statistics Workshop*, October 2015, Louvain-la-Neuve (Belgium).

4. Harnessing the complexity of MS metabolomic data: From raw signals to biomarkers. *4th Danish Symposium on Metabolomics,* November 2013, Copenhagen (Denmark).

3. Réduction de la dimensionnalité dans le cadre de l'analyse de données LC-MS. *Club Lyonnais de Chromatographie,* May 2012, Lyon (France).

2. Analysis and integration of multiple data sources in metabolomics. *Plant Metabolomics Workshop*, April 2011, Athens (Greece).

1. Knowledge discovery in high volume LC-MS metabolomic data. *Séminaire Intégration des Données*, March 2010, Avignon (France).

POSTER COMMUNICATIONS

17. Longitudinal steroidomics of human serum by UHPLC-HRMS for testosterone abuse detection. J. Boccard, F. Ponzetto, R. Nicoli, N. Baume, T. Kuuranne, M. Saugy, S. Rudaz. *Chimiométrie XIX*, January 2018, Paris (France).

16. Profilage stéroïdomique des perturbateurs endocriniens : décomposition des sources de variabilité à l'aide de la chimiométrie. J. Boccard, D. Tonoli, P. Strajhar, F. Jeanneret, A. Odermatt, S. Rudaz. *12ème Congrès de l'Association Francophone des Sciences Séparatives*, March 2017, Paris (France).

15. Multifactorial steroidomic footprinting for in vitro endocrine disruptor evaluation. J. Boccard, D. Tonoli, P. Strajhar, F. Jeanneret, A. Odermatt, S. Rudaz. *Chimiométrie XVIII*, January 2017, Paris (France).

14. Simultaneous analysis of the spatial and temporal response to wounding in *Arabidopsis thaliana* using multifactorial metabolomics and chemometrics. J. Boccard, S. Rudaz. *10èmes Journées Scientifiques du Réseau Français de Métabolomique et Fluxomique*, June 2016, Montpellier (France).

13. Analyse métabolomique pour la recherche de biomarqueurs urinaires d'exposition à la dioxine chez l'Homme. J. Boccard, F. Jeanneret, D. Tonoli, F. Badoud, O. Sorg, J.-H. Saurat, D. Hochstrasser, S. Rudaz. *Chimiométrie XV*, September 2013, Brest (France).

12. Discovery of biomarkers of dioxin intoxication in human urine: analysis by metabolomics and biologically-driven strategy. J. Boccard, F. Jeanneret, O. Sorg, J.-H. Saurat, S. Vlckova, D. Pelclova, D.N. Rutledge, D. Hochstrasser, S. Rudaz. *Eurotox*, September 2013, Interlaken (Switzerland).

11. Metabolomics applied to dioxin intoxication: biologically-driven strategy for the discovery of biomarkers in human urine. J. Boccard, F. Jeanneret, O. Sorg, J.-H. Saurat, D. Pelclova, D.N. Rutledge, D. Hochstrasser, S. Rudaz. *Systems Toxicology*. April-May 2013, Ascona (Switzerland).

10. Iterative weighting of multiblock data in the OPLS framework. J. Boccard, D.N. Rutledge. *AfroData*, November 2012, Stellenbosch (South Africa).

9. From targeted to extended steroid profile for doping analysis. J. Boccard, F. Badoud, E. Grata, S. Ouertani, M. Hanafi, G. Mazerolles, P. Lantéri, J.-L. Veuthey, M. Saugy, S. Rudaz. *Chimiométrie XII*, December 2010, Paris (France).

8. Machine learning applied to UPLC-TOF/MS metabolic fingerprinting for the discovery of wound markers in *Arabidopsis thaliana*. J. Boccard, S. Rudaz, A. Kalousis, M. Hilario, P.-A. Carrupt, J.-L. Veuthey, J.-L. Wolfender. *Fall Meeting of the Swiss Chemical Society*, September 2009, EPFL, Lausanne (Suisse).

7. Multiway 3D solvatochromic analysis of molecular interaction forces between flavonoid derivatives and P glycoprotein. J. Boccard, F. Bajot, E. Nicolle, A. Boumendjel, S. Rudaz, P.-A. Carrupt. *Fall Meeting of the Swiss Chemical Society*, September 2007, EPFL, Lausanne (Suisse).

6. Multiway PLS calibration based on 3D solvatochromic descriptors with artificial membrane PAMPA-skin experimental data. J. Boccard, G. Ottaviani, S. Martel, S. Rudaz, P.-A. Carrupt. *GGMM*, May 2007, Autrans (France).

5. Analyse multivariée par OSC-ACP/CAH de données métabolomiques obtenues par HPLC-TOF/MS chez *A. thaliana*. J. Boccard, E. Grata, G. Glauser, P.-A. Carrupt, J.-Y. Gauvrit, P. Lantéri, J.-L. Wolfender, S. Rudaz. *Chimiométrie VIII*, November 2006, Paris (France).

4. Chemometric analysis of LC-TOF/MS metabolomic data from wounded *Arabidopsis thaliana* specimens. J. Boccard, E. Grata, G. Glauser, P.-A. Carrupt, J.-Y. Gauvrit, P. Lantéri, J.-L. Wolfender, S. Rudaz. *Rencontre des Sciences Pharmaceutiques de l'Arc Alpin*, November 2006, Archamps (France).

3. Stress biomarkers discovery in *Arabidopsis thaliana* after wounding based on rapid LC-TOF/MS experiments. J. Boccard, E. Grata, G. Glauser, P.-A. Carrupt, J.-Y. Gauvrit, P. Lantéri, J.-L. Wolfender, S. Rudaz. *Fall Meeting of the Swiss Chemical Society*, October 2006, Zurich (Suisse).

2. Multivariate analysis of metabolomic data from *Arabidopsis thaliana* stressed by wounding with rapid LC/TOF-MS and gradient LC/quadrupole-MS analysis. J. Boccard, E. Grata, C. Didon, A. Thiocone, P.-A. Carrupt, J.-L. Wolfender, S. Rudaz. *Fall Meeting of the Swiss Chemical Society*, October 2005, Lausanne (Suisse).

1. Visualisation et comparaison de données obtenues par LC-APCI-MS dans le cadre d'une étude métabolomique chez *A. thaliana*. J. Boccard, E. Grata, A. Thiocone, M. Muller, P.-A. Carrupt, J.-L. Wolfender, S. Rudaz. *Chimiométrie VI*, November 2004, Paris (France).

AWARDS AND DISTINCTIONS

15. Best flash presentation, 1st prize. **Biosource-guided network annotation and visualization for untargeted metabolomics.** S. Codesido, V. González-Ruiz, E. Olesti, J. Boccard, S. Rudaz. *RFMF-Metabomeeting*, January 2020, Toulouse (France).

14. Best poster award, 2nd prize. **Metabolomics in Chronic Kidney Disease: Toward a Better Understanding of Disease Progression and Hemodialysis.** Y. Gagnebin, J. Pezzatti, P. Lescuyer, S. De Seigneux, J. Boccard, S. Rudaz, B. Ponte, 32nd *International Symposium on Chromatography*, September 2018, Cannes (France).

13. Best poster award, 3rd prize. **Metabolomic analysis of urine samples by UHPLC-QTOF-MS: impact of normalization strategies.** Y. Gagnebin, D. Tonoli, P. Lescuyer, B. Ponte, S. De Seigneux, P.-Y. Martin, J. Schappler, J. Boccard, S. Rudaz, *27th International Symposium on Pharmaceutical and Biomedical Analysis*, November 2016, Guangzhou (China).

12. Best poster award (Phytochemical Society of Europe), 1st prize. **Detection and dynamics of volatile/non-volatile metabolite induction in fungal co-culture through a miniaturised MS-based metabolomic approach.** A. Azzollini, L. Boggia, J. Boccard, B. Sgorbini, N. Lecoutre, P. Rubiolo, S. Rudaz, K. Gindro, C. Bicchi, J.-L. Wolfender, *9th Joint Natural Products Conference*, July 2016, Copenhagen (Denmark).

11. Best poster award, 1st prize. **Suivi longitudinal de stéroïdes endogènes dans le sérum humain par UHPLC-MS/MS comme outil de détection de l'usage de testostérone dans le sport.** F. Mehl, F. Ponzetto, R. Nicoli, N. Baume, M. Saugy, J. Boccard, S. Rudaz. *Chimiométrie XVII*, January 2016, Namur (Belgium).

10. Best poster award, 1st prize. **Analyse métabolomique de l'urine : stratégies de normalisation en UHPLC-QTOF-MS.** Y. Gagnebin, J. Schappler, J. Boccard, S. Rudaz *Chimiométrie XVI*, January 2015, Geneva (Switzerland).

9. Journal Highlight in spectroscopyNOW (Chemometrics & Informatics), February-March 2014. **Harnessing the complexity of metabolomic data with chemometrics**. J. Boccard, S. Rudaz. *Journal of Chemometrics* (2014), 28(1), 1-9.

8. Best poster award, 2nd prize. **Analyse métabolomique pour la recherche de biomarqueurs urinaires d'exposition à la dioxine chez l'Homme.** J. Boccard, F. Jeanneret, D. Tonoli, F. Badoud, O. Sorg, J.-H. Saurat, D. Hochstrasser, S. Rudaz. *Chimiométrie 2013*, September 2013, Brest (France).

7. Best poster communication for spectroscopic techniques **(**Brucker), 1st prize. **Analyse multi-tableaux de données UHPLC-QTOF-MS, RMN et FT-MIR : application à la différentiation d'huile essentielle de citron,** F. Mehl, G. Marti, J. Boccard, L. Marcourt, B. Debrus, P. Merle, E. Delort, L. Baroux, H. Sommer, J.-L. Wolfender, S. Rudaz. *Chimiométrie 2011*, December 2011, Marseille (France)

6. Best poster award, 2nd prize. **Profiling of endogenous steroids by UHPLC-QTOF-MS^E,** F. Badoud, E. Grata, J. Boccard, S. Rudaz, J.-L. Veuthey, M. Saugy. *Congress on Steroid Research*, March 2011, Chicago (USA).

5. Top 25 Hottest articles, October to December 2011, January to March 2012 & January to December 2012 full year, *Forensic Science International*. **Analytical aspects in doping control: Challenges and perspectives**. F. Badoud, D. Guillarme, J. Boccard, E. Grata, M. Saugy, S. Rudaz, J.-L. Veuthey. *Forensic Science International*. (2011), 213(1-3), 49-61.

4. Top 25 Hottest articles, October to December 2010 & January to March 2011, *Chemometrics and Intelligent Laboratory Systems*. **Standard machine learning algorithms applied to UPLC-TOF/MS metabolic fingerprinting for the discovery of wound biomarkers in *Arabidopsis thaliana***. J. Boccard, A. Kalousis, M. Hilario, P. Lanteri, M. Hanafi, G. Mazerolles, J.-L. Wolfender, P.-A. Carrupt, S. Rudaz. *Chemometrics and Intelligent Laboratory Systems* (2010), 104(1), 20-27.

3. Best poster award, 1st prize, **Analyse stéroïdomique dans l'urine par UHPLC-QTOF-MS pour le dépistage anti-dopage,** J. Boccard, F. Badoud, E. Grata, S.S. Ouertani, M. Hanafi, G. Mazerolles, P. Lantéri, J.-L. Veuthey, M. Saugy, S. Rudaz *Chimiométrie 2010*, December 2010, Paris (France).

2. Hottest Articles in Analytical Chemistry / Top accessed articles during 2010, *Journal of Separation Science*. **Knowledge discovery in metabolomics: an overview of MS data handling**. J. Boccard, J.-L. Veuthey, S. Rudaz. *Journal of Separation Science* (2010), 33(3), 290-304.

1. Top 25 Hottest articles, April to June 2007 & July to September 2007, *Chemometrics and Intelligent Laboratory Systems*. **Multivariate data analysis of rapid LC-TOF/MS experiments from *Arabidopsis thaliana* stressed by wounding**. J. Boccard, E. Grata, A. Thiocone, J.-Y. Gauvrit, P. Lanteri, P.-A. Carrupt, J.-L. Wolfender, S. Rudaz. *Chemometrics and Intelligent Laboratory Systems* (2007), 86(2), 189-197.

HONORS

INVITED PROFESSOR

1. University of Picardy Jules Verne, 2018, Amiens (France).

SCIENTIFIC ADVISORY BOARDS

1. MEtabolomics LIpidomics Steroidomics Analysis (MELISA) Platform (since 2017). Laboratoire d'Etude des Résidus et Contaminants dans les Aliments (LABERCA), ONIRIS, Nantes (France).

2. Polyphenols Platform (since 2019), INRAe & SupAgro, Montpellier (France).

PHD SUPERVISIONS

1. Yoric Gagnebin (2014-2019). **Multiplatform metabolomic characterization of biofluids**. Co-direction Prof. S. Rudaz, University of Geneva (Switzerland).

PHD JURIES

8. Nicolas Di Giovanni. **Development of multidimensional approaches for metabolomics** (2021). Scientific direction: J.-F. Focant, Liège University (Belgium).

7. Céline Dalle. **Profilage lipidomique ciblé des oxylipines pour identifier de nouveaux biomarqueurs du syndrome cardiométabolique - Robustesse analytique et pertinence biologique** (2020). Scientific direction: C. Gladine, Clermont Auvergne University (France).

6. Hikmat Ghosson. **Développement d'un nouveau proxy universel pour évaluer le devenir et l'impact environnemental de (bio)pesticides complexes par Métabolomique basée sur la Spectrométrie de Masse** (2020). Scientific direction: C. Bertrand and M.-V. Salvia, University of Perpignan Via Domitia (France).

5. Julian Pezzatti. **Application and evaluation of liquid chromatography – high resolution mass spectrometry in untargeted metabolomics for compound annotations in biological matrices** (2020). Scientific direction: S. Rudaz, University of Geneva (Switzerland).

4. Oriane Moyne. **Approche métabolomique pour l'étude de l'évolution adaptative de Pseudomonas aeruginosa au cours des infections pulmonaires chroniques dans la mucoviscidose** (2019). Scientific direction: B. Toussaint and D. Bicout, Grenoble Alpes University, (France).

3. Baninia Habchi. **Mise en évidence des perturbations métaboliques liées à l'exposition aux toxiques présents dans l'environnement ou l'aliment par spectrométrie de masse à ultra haute résolution FTMS combinée avec des outils chimiométriques** (2017). Scientific direction: E. Rathahao-Paris and S. Alves, Paris-Saclay University, Paris (France).

2. Samar Azzi Achtouky. **Etude de l'évolution du profil aromatique des moûts de Syrah issus de deux régions libanaises au cours de la fermentation par analyse GC-MS et Chimiométrie** (2014). Scientific direction: D. Rutledge, AgroParisTech, Paris (France) and N. Ouaini, Holy Spirit University of Kaslik, Beirut, (Lebanon).

1. Samia Samar Ouertani. **Méthodologie statistique pour un traitement différentiel des données métaboliques** (2014). Scientific direction: M. Hanafi, ONIRIS, Nantes (France) and S. Rudaz, University of Geneva (Switzerland).

PHD COMMITTEES

7. Maxime Delmas. **Prédiction d'effets pathologiques liés à l'exposition à des xénobiotiques par comparaison de signatures métaboliques** (2020). Scientific direction: F. Jourdan and C. Frainay, Université Toulouse III - Paul Sabatier, Toulouse (France).

6. Denis Werner. **Infférence de source de traces d'essence : étude de la contribution combinée des compositions moléculaire et isotopique** (2019). Scientific direction: O. Delémont, University of Lausanne, Lausanne (Suisse).

5. Katy Dinis. **Development of new applications in food authenticity analysis by Liquid Chromatography coupled to High Resolution Mass Spectrometry** (2019 & 2020). Scientific direction: V. Camel, AgroParisTech, Paris (France) and F. Thomas, Eurofins, Nantes (France).

4. Thibaut Dumas. **Investigation des effets de contaminants émergents chez le bivalve marin *Mytilus galloprovincialis* à travers l'approche métabolomique** (2018 & 2019). Scientific direction: F. Courant and E. Gomez, University of Montpellier, Montpellier (France).

3. Stéphanie Monnerie. **Apport de la modélisation pour une meilleure stratification des populations à risque – Application à la caractérisation du syndrome métabolique chez la personne âgée** (2018 & 2019). Scientific direction: E. Pujos-Guillot, INRAe, Clermont-Ferrand (France) and P. Gaudreau, University of Montréal, Montréal (Canada).

2. Jihéne Bouhlel. **Determination of volatile organic compounds as markers to back trace food chain exposure to micropollutants** (2016). Scientific direction: E. Engel, INRAe, Clermont-Ferrand (France) and D. Rutledge, AgroParisTech, Paris (France).

1. Bénédict Yanibada. **Recherche de marqueurs de la production de méthane chez la vache laitière par une approche métabolomique multiplateforme** (2015 & 2017). Scientific direction: H. Boudra and D. Morgavi, INRAe, Clermont-Ferrand (France).

MASTER SUPERVISIONS

2. Marion Brandolini-Bunlon. **Comparaison d'analyses multi-blocs pour l'intégration de données métabolomiques et épidémiologiques** (2017). Clermont Auvergne University (France)

1. Eva-Marie Golder. **Prédiction du temps de rétention des stéroïdes glucuroconjugués** (2016). University of Geneva (Switzerland).

MASTER JURIES

2. René Nellen. **Simultaneous determination of progestins and steroid profiles in plasma by HPLC-MS** (2018). Scientific direction: H. Henry, University of Lausanne (Switzerland).

1. Vadym Mozgovoy. **Metropolis-Hastings MCMC for univariate and bivariate Bayesian Lasso Regression in the steroid detection context** (2017). Scientific direction: M.-O. Boldi, University of Geneva (Switzerland).